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NUMERICAL SOLUTION OF SECOND ORDER DIFFERENTIAL EQUATIONS USING RATIONAL PADE CONVERGENTS

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NUMERICAL SOLUTION OF SECOND ORDER

DIFFERENTIAL EQUATIONS USING RATIONAL PADÉ CONVERGENTS

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William B. Moye, Jr.

NUMERICAL SOLUTION OF SECOND ORDER DIFFERENTIAL EQUATIONS USING RATIONAL PADÉ COEFFICIENTS

by

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Lieutenant Commander, United States Navy

Submitted in partial fulfillment of
the requirements for the degree of

MASTER OF SCIENCE

United States Naval Postgraduate School
Monterey, California

1966

NUMERICAL SOLUTION OF SECOND ORDER

DIFFERENTIAL EQUATIONS USING RATIONAL FACE CONVERGENTS

by

William B. Hope, Jr.

This work is accepted as Fulfilling
the thesis requirements for the degree of

MASTER OF SCIENCE

from the

United States Naval Postgraduate School

ABSTRACT

Rational Padé convergents to a function of the forward shift operator E are computed from coefficients of its power series expansion. These Padé convergents are used to generate recursion formulas which are then employed to obtain approximate numerical solutions of several second order differential equations. A variety of integration step lengths are used. Solution error is plotted against the number of iteration steps and results are evaluated. It is concluded that this procedure is beneficial as a method of deriving corrector formulas to be used in the predictor-corrector method of solving second order differential equations. A method for deriving improved predictor formulas is suggested.

ACKNOWLEDGEMENTS

This project was suggested by Professor U. K. Kadres of the U. S. Naval Postgraduate School, to whom the writer is indebted for much valuable assistance.

Gratitude is also expressed to Professor R. J. Stewart who read the manuscript and offered a number of helpful suggestions.

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1. Introduction.

Lyusternik [3] has suggested a numerical method for solving differential equations which uses rational Pade convergents to approximate functions of the forward shift operator E to generate recursion formulas. He has demonstrated the merits of using such formulas in solving first order equations and has exhibited certain stability problems related thereto.

The purpose of this paper is to extend the study of this method in the special category of second order differential equations in which the first derivative does not appear. A computer program is developed which generates a number of recursion formulas, applies them successively to solve the initial value problem $y'' + y = 0$, $y(0) = 1$, $y'(0) = 0$, and produces graphs of solution error vs number of iterations. The basic program is then modified to solve the Coulomb Wave Equation $y'' + y\left(1 - \frac{2\eta}{x} - \frac{L(L+1)}{x^2}\right) = 0$ with initial conditions appropriate to the selected values of the parameters η and L. The Runge-Kutta method is used to compute eight values of the independent variable to start the solution. Finally, the results of these computations are discussed in detail.

Some of the advantages of this method over others in common use are:

a. A rational convergent is generally a better approximation to a function than is the corresponding truncated series. This will be discussed further in the following section.

b. Only about one half the total number of tabular differences required by methods using polynomial approximations are needed in this method for comparable accuracy. This is because differences are distributed over both sides of the recursion formula.

c. Since differencing is divided between both sides of the

equation, neither side is differenced too many times. This reduces the number of computations required and, consequently, the round off error.

4. Recursion formulas derived from Field convergents are extremely easy to generate in a digital computer program. This will be illustrated in Section 4.

2. Derivation of Rectangular Formulas.

Suppose it is desired to solve the initial value problem

$$y''(x) = f(x, y(x)), \quad y(x_0) = y_0, \quad y'(x_0) = y'_0. \tag{1}$$

Integrating formally on each side

$$\int_{x_0}^{x_0+h} \int_{x_0}^{x} y''(\xi)\, d\xi\, dt = \int_{x_0}^{x_0+h} \int_{x_0}^{t} f(\xi, y(\xi))\, d\xi\, dt$$

we get on the left side

$$\int_{x_0}^{x_0+h} [y'(x) - y'(x_0)]\, dt = y(x_0+h) - y(x_0) - y'(x_0)h.$$

Introducing a change of variable

$$\xi = x_0 + hs_1, \qquad d\xi = h\,ds_1$$

$$t = x_0 + hs_2, \qquad dt = h\,ds_2$$

and defining the forward shift operator E such that $E^n f(x) = f(x+nh)$, we get on the right (treating E as an algebraic symbol):

$$h^2 \int_0^1 \int_0^{s_2} f(x_0 + hs_1, y(x_0 + hs_1))\, ds_1\, ds_2 = h^2 \int_0^1 \int_0^{s_2} E^{s_1} f(x_0)\, ds_1\, ds_2$$

$$= h^2 \int_0^1 \left[\frac{E^{s_2} - 1}{\log E} \right] f(x_0)\, ds_2 = \frac{h^2}{\log E} \int_0^1 (E^{s_2} - 1) f(x_0)\, ds_2 = \frac{h^2}{\log E} \left\{ \left[\frac{E^{s_2}}{\log E} - s_2 \right]_0^1 \right\} f(x_0)$$

$$= \frac{h^2}{\log E} \left\{ \frac{E}{\log E} - 1 \right\} f(x_0) = \frac{h^2}{\log E} \left\{ \frac{E-1}{\log E} - 1 \right\} f(x_0).$$

Finally,

$$y_1 - y_0 - hy'_0 = \left(\frac{h}{\log E} \right)^2 \left\{ \frac{E-1}{\log E} - 1 \right\} f_0$$

or,

$$y_1 = y_0 + hy'_0 + \left(\frac{1}{\log E} \right)^2 \left\{ \frac{E-1}{\log E} - \frac{h}{\log E} \right\} f_0.$$

Assuming we know y_i $i=1,\dots,n$ we can write

$$y_{n+1} = \left(\frac{h}{\log\epsilon}\right)^2 f_{n-1} + y_n + h(\epsilon-1)y_n' - \left(\frac{h}{\log\epsilon}\right)^2 \left\{ h \cdot [1-\dots] f_n \right\}$$

Setting $i = 1$ $\quad y_{n+1} - y_n = \left(\frac{h}{\log\epsilon}\right)^2 \left\{ f_{n+1} - f_n \right\} + h y_n' - \frac{h^2}{\log\epsilon} f_n + \dots$

$$(\epsilon-1)y_n = \left(\frac{h}{\log\epsilon}\right)^2 (\epsilon-1) f_n + h y_n' - \frac{h^2}{\log\epsilon} f_0, \quad y_n = \left(\frac{h}{\log\epsilon}\right)^2 f_n + \frac{h}{\epsilon-1} y_n' - \frac{h^2 f_0}{\log\epsilon\,(\epsilon-1)}.$$

In terms of the backward difference operator ∇, defined by $\nabla y_i = y_i - y_{i-1}$, this is

$$y_n = \left\{ \frac{h}{-\log(1-\nabla)} \right\}^2 f_n + h \frac{(1-\nabla)}{\nabla} y_n' - \frac{h^2}{-\log(1-\nabla)} \cdot \frac{(1-\nabla)}{\nabla} f_0.$$

Multiplying through by ∇^2

$$\nabla^2 y_n = \left\{ \frac{h}{\log(1-\nabla)} \right\}^2 f_n + h(\nabla-\nabla^2) y_n' + \frac{h}{\log(1-\nabla)} \cdot (\nabla-\nabla^2) f_0 = \left\{ \frac{h}{\log(1-\nabla)} \right\}^2 f_n$$

since ∇ operating on a constant yields zero.

For simplicity of notation we let $z_i = \nabla^2 y_i$ and write

$$z_i = \left\{ \frac{h}{\log(1-\nabla)} \right\}^2 f_i \qquad (1)$$

Let $a_0 + a_1\nabla + a_2\nabla^2 + \dots$ be the power series expansion of $\left\{ \frac{h}{\log(1-\nabla)} \right\}^2$. The power series can be approximated by a rational fraction by use of the following technique. $a_0 + a_1\nabla + a_2\nabla^2 + \dots + a_n\nabla^n \simeq \frac{b_0 + b_1\nabla + \dots + b_p\nabla^p}{1 + c_1\nabla + \dots + c_q\nabla^q}$. Multiplying each side by the denominator of the above fraction and equating coefficients of the like power terms in ∇ we generate $p+q+1$ linear equations in the $p+q+1$ unknowns $b_0 \dots b_p$, $c_1 \dots c_q$.

$$\begin{aligned} b_0 &= a_0 \\ b_1 &= a_1 + a_0 c_1 \\ b_2 &= a_2 + a_1 c_1 + a_0 c_2 \\ b_3 &= a_3 + a_2 c_1 + a_1 c_2 + a_0 c_3 \\ &\vdots \end{aligned}$$

The solution of this system gives us the coefficients of the rational fraction which agrees with the series out to $p+q+1$ terms.

It should be noted that a given polynomial of degree r can be equated

identically to each of r + 1 distinct fractions. Truncating the polynomial after 1, 2, ..., n terms, successively, we obtain a collection of polynomial fractions which can be arranged as a Padé table of rational convergents. Fig. 1 is the Padé table associated with $\left\{\frac{\log(1-\nabla)}{\nabla}\right\}^2$ where a third degree polynomial is used to generate the rational convergents.

The power series expansion of $\left\{\frac{\log(1-\nabla)}{\nabla}\right\}^2$, truncated to seven terms, is the sixth degree polynomial

$$1 + \nabla + \frac{11}{12}\nabla^2 + \frac{5}{6}\nabla^3 + \frac{137}{180}\nabla^4 + \frac{7}{10}\nabla^5 + \frac{363}{560}\nabla^6. \qquad (3)$$

The coefficients of this polynomial were used as inputs to Program E UCSD PADÉ (Naval Postgraduate School Library Routine) to obtain coefficients of the 26 Padé convergents whose numerators and denominators are polynomials of degree q and p, respectively, and where $p+q \leq 6$. Fig. 2 lists these coefficients, rounded to three significant figures.

As stated above, each of these convergents is identically equal to (3) out to p+q+1 terms. Moreover, a given convergent expanded algebraically into a power series generally continues to agree quite well with the related infinite series for a number of terms beyond the $(p+q+1)^{st}$; i.e., a rational convergent generally is a better approximation to a function than is the truncated series from which the convergent was derived.

Designate a particular convergent to $\left\{\frac{\log(1-\nabla)}{\nabla}\right\}^2$ by

$$\frac{A_0 + A_1\nabla + A_2\nabla^2 + \cdots + A_p\nabla^p}{B_0 + B_1\nabla + B_2\nabla^2 + \cdots + B_q\nabla^q}. \qquad (4)$$

Suppose we wish to find an approximate numerical solution of the equation $y'' = f(x,y)$. Substituting (4) for $\left\{\frac{\log(1-\nabla)}{\nabla}\right\}^2$ in equation (2) we have

$$z_1 = h^2 f_1 \Big/ \left(\frac{A_0 + A_1\nabla + \cdots + A_p\nabla^p}{B_0 + B_1\nabla + \cdots + B_q\nabla^q}\right).$$

Simplifying, this becomes $(A_0 + A_1\nabla + \cdots + A_p\nabla^p)z_1 = h^2(B_0 + B_1\nabla + \cdots + B_q\nabla^q)f_1$.

Setting $\nabla^2 y_i = \frac{\partial^2}{\partial x^2} \ldots$, we can express the above equation in the form [illegible] (5)

Denote the coefficients in (5) as follows:

$$Q(j) = \sum_{i=1}^{q} \binom{i}{j} AB(i+1)$$

$$P(j) = \sum_{i=1}^{p} \binom{i}{j} AD(i+1)$$

Substituting the coefficients in (5) we have:

$$Q(0)z_i - Q(1)z_{i-1} + \ldots \pm Q(q)z_{i-q} = h^2\left[P(0)f_i - P(1)f_{i-1} + \ldots \pm P(p)f_{i-p}\right], \text{ or,}$$

$$z_i = \frac{1}{AB(1)}\left\{Q(1)z_{i-1} - \ldots \pm Q(q)z_{i-q} + h^2\left[P(0)f_i - \ldots \pm P(p)f_{i-p}\right]\right\}. \qquad (6)$$

Here z_i is given in terms of coefficients of the Padé convergent and of previously computed values of z and f. Recalling that $z_i = \nabla^2 y_i = y_i - 2y_{i-1} + y_{i-2}$ we may now calculate $y_i = z_i + 2y_{i-1} - y_{i-2}$. The value of f_i used in (6) will have been computed from a first approximation to y_i generated by a predictor formula.

3. Stability Considerations.

The recursion formula generated from a given Padé convergent is of the form $Q(0)z_i = Q(1)z_{i-1} - \ldots \pm Q(q)z_{i-q} + h^2\left[P(0)f_i - \ldots \pm P(p)f_{i-p}\right]$, (7) where Q(i) and P(i) are as defined in Section 2.

Substituting $\nabla^2 y_i = y_i - 2y_{i-1} + y_{i-2}$ for z_i in (7) we obtain

$$Q(0)\,(y_i - 2y_{i-1} + y_{i-2}) + Q(1)\,(y_{i-1} - 2y_{i-2} + y_{i-3}) - \ldots \pm Q(q)\,(y_{i-q} - 2y_{i-q-1} + y_{i-q-2}) = h^2\left[P(0)f_i - P(1)f_{i-1} + \ldots \pm P(p)f_{i-p}\right]$$

Multiplying and collecting terms, this becomes

$$Q(0)y_i - \left[Q(1) + 2Q(0)\right]y_{i-1} + \left[Q(2) + 2Q(1) + Q(0)\right]y_{i-2} + \ldots$$
$$+ (-1)^{q+1}\left[Q(q) + 2Q(q-1) + Q(q-2)\right]y_{i-q} + (-1)^{q}\left[2Q(q) + Q(q-1)\right]y_{i-q-1}$$
$$+ (-1)^{q-1}Q(q)y_{i-q-2} + h^2\left[P(0)f_i - \ldots + (-1)^{p}P(p)f_{i-p}\right] \qquad (8)$$

The general solution of this difference equation is of the form

$y_n = c_1 r_1^n + c_2 r_2^n + \ldots + c_k r_k^n$ where $r_1, r_2, \ldots, r_k$ are roots of the associated characteristic equation (to be introduced later) and the c_i are constants.

Consider the 2nd order Padé convergent $\frac{1}{1 - \sigma + \frac{1}{12}\sigma^2}$ (Formula 1 in Fig.). From the discussion of Section 2 we know that the recursion formula generated by this convergent will have the following coefficients:

$$Q(0) = 1; \quad Q(i) = 0, \; i \geq 1$$

$$P(0) = \tfrac{1}{12}; \; P(1) = -\tfrac{10}{12}; \; P(2) = \tfrac{1}{12}; \; P(i) = 0, \; i \geq 3$$

The general recursion formula (8) then becomes

$$y_i = 2y_{i-1} - y_{i-2} + h^2\left[\tfrac{1}{12} f_i + \tfrac{10}{12} f_{i-1} + \tfrac{1}{12} f_{i-2}\right]. \qquad (9)$$

In the initial value problem (1) it is seen that $f_i = -y_i$. Substituting in (9) and collecting terms:

$$(1 + \tfrac{1}{12}h^2)y_i = (2 - \tfrac{10}{12}h^2)y_{i-1} - (1 + \tfrac{1}{12}h^2)y_{i-2}$$

or,

$$(12+h^2)y_i - (24-10h^2)y_{i-1} + (12+h^2)y_{i-2} = 0$$

Finding roots: $$\sim = \frac{(24-10h^2) \pm \sqrt{(24-10h^2)^2 - 4(12+h^2)^2}}{2(12+h^2)}$$

$$= \frac{(12-5h^2) \pm ih\sqrt{144 - 24h^2}}{12+h^2} \qquad (10)$$

Ignoring terms of the order of h^2 we have

$$\sim \simeq \frac{12 + 12ih}{12} = 1 \pm ih \qquad (11)$$

The general solution of (9) is of the form

$$y_n \simeq c_1 r_1^n + c_2 r_2^n$$

We determine the coefficients c_i from the solution $y = \cos x$ of the initial value problem.

$y_0 = c_1 r_1^0 + c_2 r_2^0 = 1$ (initial conditions give $y_0 = 1$)

$y_1 = c_1 r_1 + c_2 r_2 = 1 - \frac{h^2}{2}$ ($y = \cos h = 1 - \frac{h^2}{2} + \frac{h^4}{4!} \ldots$. For small values of h, $1 - \frac{h^2}{2}$ is a good approximation)

Solving these equations simultaneously:

$$A_1 = \frac{2+h}{4i} \quad , \quad A_2 = \frac{2-h}{4i}$$

Thus we have:

$$y_n = \frac{2-h}{4i}(1+h^2)^n + \frac{2+h}{4i}(1-h^2)^n \qquad (12)$$

This can be written in trigonometric form:

$$y_n = \left(\frac{1}{2}+\frac{h}{4}i\right)\left[\left(\sqrt{1+h^2}\right)^n(\cos n\theta + i\sin n\theta)\right] + \left(\frac{1}{2}-\frac{h}{4}i\right)\left[\left(\sqrt{1+h^2}\right)^n(\cos n\theta - i\sin n\theta)\right]$$

where $\theta = \arcsin \frac{h}{\sqrt{1+h^2}}$.

$$y_n = \left(\sqrt{1+h^2}\right)^n\left\{\left(\frac{1}{2}+\frac{h}{4}i\right)(\cos n\theta + i\sin n\theta) + \left(\frac{1}{2}-\frac{h}{4}i\right)(\cos n\theta - i\sin n\theta)\right\}$$

$$= \left(\sqrt{1+h^2}\right)^n\left(\cos n\theta - \frac{h}{2}\sin n\theta\right) \qquad (13)$$

for small h, $h \simeq \theta$, in which case

$$y_n \simeq \left(\sqrt{1+h^2}\right)^n\left(\cos nh - \frac{h}{2}\sin nh\right)$$

and this solution converges to the exact solution.

It can be seen from the graphs that Formulas 10, 11, 12, 15, 23, and 25 are the most promising from the standpoint of minimum error amplification. Unfortunately, their associated characteristic equations (fourth through seventh degree) are too intractable to permit analysis. It would be quite simple, however, to obtain the roots of these equations with an appropriate computer program. The error characteristics of the equations could then be determined from a study of the properties of their roots. This is discussed in Section 7 as a project recommended for future study.

The foregoing paragraphs were concerned with the accumulation of truncation error without regard for the fact that errors in y_{n-1} and y_{n-2} in (4) will affect subsequent errors. To consider this effect a different approach will be taken.

In terms of the difference equation (9),

$$\bar{y}_i = \bar{y}_{i-1} + h\left[\frac{1}{12}\bar{f}_i + \frac{10}{12}\bar{f}_{i-1} - \frac{1}{12}\bar{f}_{i-2}\right] + T(h) + R(i) \qquad (14)$$

where $\bar{y}_i$ is the value of solution of the initial value problem at x_i, and $\bar{f}_i = f(x_i, \bar{y}_i)$. $T(h)$ is the truncation error introduced by using $\frac{1}{1-0.5z^{-1}}$ to approximate $\left\{\frac{\ln(1+z)}{z}\right\}^{-1}$, and $R(i)$ is the roundoff error. We define $E(h,i) = T(h) + R(i)$.

Defining $\epsilon_i = \bar{y}_i - y_i$, we subtract (9) from (14) and obtain

$$\epsilon_i = 2\epsilon_{i-1} - \epsilon_{i-2} + h\left[\frac{1}{12}(\bar{f}_i - f_i) + \frac{10}{12}(\bar{f}_{i-1} - f_{i-1}) + \frac{1}{12}(\bar{f}_{i-2} - f_{i-2})\right] + E(h,i).$$

Assuming that $f_j(x_i, y)$ is differentiable with respect to y in the interval $(\bar{y}_i, y_i)$ we may use the mean value theorem to write:

$$(\bar{f}_i - f_i) = f_y(x_i, \xi_i)(\bar{y}_i - y_i) = \epsilon_i f_y(x_i, \xi_i).$$

If $f_y(x_i, \xi_i)$ does not vary greatly we may let $f_y(x_i, \xi_i) = K$ and write

$$\epsilon_i = 2\epsilon_{i-1} - \epsilon_{i-2} + h^2K\left[\frac{1}{12}\epsilon_i + \frac{10}{12}\epsilon_{i-1} + \frac{1}{12}\epsilon_{i-2}\right] + E(h,i).$$

Collecting terms: $(1 - \frac{1}{12}h^2K)\epsilon_i = (2 + \frac{10}{12}h^2K)\epsilon_{i-1} - (1 - \frac{1}{12}h^2K)\epsilon_{i-2} + E(i,h)$

or, $(12 - h^2K)\epsilon_i = (24 + 10h^2K)\epsilon_{i-1} - (12 - h^2K)\epsilon_{i-2} + E(i,h)$.

In the solution of the initial value problem (1), $K = f_y(x_i, \xi_i) = -1$. Hence, $(12+h^2)\epsilon_i = (24-10h^2)\epsilon_{i-1} - (12+h^2)\epsilon_{i-2} + E(h,i)$. (15)

Under the assumption that $E(h,i)$ is relatively insensitive with respect to i, we may proceed as we did in solving (9). (As applied to this case the truncation error $T(h) = Ch^4y^{(4)}(\xi_i)$, and $y^{(4)}(\xi_i)$ varies slowly when the h increments are small). We will henceforth assume $E(h,i)$ to be a constant: Dh^4.

We must solve $(12 + h^2)\epsilon_i = (24-10h^2)\epsilon_{i-1} - (12+h^2)\epsilon_{i-2} + Dh^4$
$\epsilon_0 = 0$ (no error initially), and
$\epsilon_1 = \delta$ (assumed to be non-zero)

The solution consists of the general solution corresponding to the homogeneous part $\epsilon_i = c_1 r_1^i + c_2 r_2^i$ and a particular solution [illegible]

pending to the non-homogeneous part Dh^2. The particular solution can be found by assuming that ϵ_n is a constant A, so that

$(12+6^2)A = (24-12^2)A - (12+6^2)A + Dh^2$. Hence,

$$A = \frac{Dh^4}{2(12+6^2)(24-\quad)} = \frac{Dh^4}{12h^4} = \frac{Dh^2}{12}.$$

The complete solution is then $\epsilon_n = c_1 r_1^n + c_2 r_2^n + \frac{D}{12}h^2$. (16)

Let $r_1 = a + ib$, $r_2 = a - ib$.

Denote $c_1 = \alpha + i\beta$, $c_2 = \alpha - i\beta$, where $\alpha = -\frac{1}{24}h^2$ and $\beta = -\frac{1}{24}\left\{\int + (a-1)\frac{D}{12}h^3\right\}$.

The solution (16) is transformed into trigonometric form by letting

$$\theta = \text{arc sin } \frac{b}{\sqrt{a^2+b^2}}$$

Then, $\epsilon_n = |r|^n (2\alpha\cos n\theta - 2\beta\sin n\theta) + \frac{D}{12}h^2$. Expanding:

$\epsilon_n = |r|^n\left\{-\frac{D}{12}h^2\cos n\theta + \frac{1}{b}\left(\int + (a-1)\frac{D}{12}h^2\right)\sin n\theta\right\} + \frac{D}{12}h^2$.

In particular, if we approximate

$$a = 1 \quad b = h \text{ , i.e., } r_1 = 1 + ih,\ r_2 = 1 - ih$$

$$\epsilon_n = (\sqrt{1+h^2})^n\left\{-\frac{D}{12}h^2\cos n\theta + \frac{1}{h}(\int \sin n\theta)\right\} + \frac{D}{12}h^2 \quad (17)$$

where $\theta = \text{arc sin } \frac{h}{\sqrt{1+h^2}}$. For small h

$$\epsilon_n \simeq (\sqrt{1+h^2})^n\left\{-\frac{D}{12}h^2\cos nh + \frac{\int}{h}\sin nh\right\} + \frac{D}{12}h^2. \quad (18)$$

This solution of the error propagation equation qualitatively explains the behavior of the experimental results displayed in Fig. 16.

a. If h is small, the sine term of $\left\{-\frac{D}{12}h^2\cos nh + \frac{\int}{h}\sin nh\right\}$ is significant and the cosine term is negligible. Error would be expected to vary nearly sinusoidally.

b. ϵ_n should be approximately equal to zero where nh is multiple of π, since the term $\frac{\int}{h}\sin nh$ will vanish at these points. Given $h = .02$ and solving for $n = \frac{k\pi}{.02}$, $k = 1, 2, \ldots, 5$, we expect to find

near-exact error where n = 157, 344, 471, 486 and 785. Fig. 16 shows this to be the case. Error nulls shown in Figs. 33 and 41 can be explained similarly by solving for n with h = .01 and .05, respectively.

c. The bracketed term in (1^n) is multiplied by $|r|^n$. Hence, the error amplitude should grow with increasing n if $|r| > 1$ and diminish if $|r| < 1$. The amplification factor $(\sqrt{1+h^2})^n$ in (18) is only an approximation of $|r|^n$. The actual roots were found to be

$$r = \frac{(12-5h^2) \pm ih\sqrt{144-24h^2}}{12+h^2}$$

$$|r|^2 = \frac{(144-120h^2+25h^4)+h^2(144-24h^2)}{144+24h^2+h^4} = 1$$

for all h. Whenever h is small enough to insure that (18) closely approximates (17), error maxima should remain nearly constant. Fig. 33 substantiates this for h = .01. Increasing error maxima in Figs. 19 and 41 (h = .02 and .05, respectively) are attributed to the failure of h to meet the criterion stated above.

No explanation is offered for the high frequency error oscillation so prevalent in some of the graphs, e.g. Fig. 16. Investigation of this phenomenon is suggested as a project for future study.

4. Description of the Test Program.

This program is designed to solve a given second order differential equation 26 times, successively using each of 26 Padé convergents to generate a central recursion formula. Integration of the given equation is by the predictor-corrector method, using the Milne predictor formula: $y_{n+1} = y_{n-3} + \frac{4h}{3}[2y'_{n-2} - y'_{n-1} + 2y'_n]$. Necessary starting values are computed by the Runge-Kutta method. The iterative process may be carried out to as many as 900 steps, solution error being

determined at each step if an exact solution of the given equation is known. Graphs are plotted with error as ordinate and number of iterations as abscissa. Fig. 3 explains the symbols used in the programs. Fig. 4 is a printout of the program used to evaluate the equation generating the cosine function, $y'' + y = 0$ (Program TMOD 2). Fig. 5 is a printout of the program used to evaluate the Coulomb Wave Equation $y'' + y\left(1 - \frac{2\eta}{r} - \frac{\ell(\ell+1)}{r^2}\right) = 0$ (Program TMOD 6).

5. Discussion of Data.

a. Program TMOD 2

(1) Figs. 7 through 25 are graphs of progressive error resulting when the initial value problem $y'' + y = 0$, $y(0) = 1$, $y'(0) = 0$ is solved using an integration step length of .02 and corrector formulas derived from the various Padé convergents. Fig. 6 relates the recursion formula number shown on each graph to a description of the corresponding Padé fraction. Formulas 16, 17, 20, 21, 23, 24 and 26 diverged rapidly and no associated graphs were plotted.

(a) Formulas 10, 11, 12, 15, 22 and 25 produced remarkable accuracy over the entire range of 900 iterations.

(b) Formula 6 (Fig. 12), although less accurate than the group just discussed, has an important property: error maxima are diminished with increasing iteration.

(c) The remaining graphs indicate that error maxima are not being damped but are increasing linearly with respect to n, the number of iterations.

(2) The second set of data was obtained by repeating the preceding experiment after decreasing the integration step length to .01.

The following were observed:

(a) The runs which proved to be most accurate with a step length of .02 (Formulas 10, 11, 13, 15, 22 and 25) were found to be less accurate with the smaller step length (contrary to what would be expected). Formulas 15, 22 and 25 show a small error amplification while all the others in this group show a much greater error amplification. Figs. 28 through 33 are graphs showing these results.

(b) Formula 6 provides less accurate results than with the greater step length but its error damping characteristics remain. (Fig. 27)

(c) Formula 5 is more stable. Its accuracy is comparable to that in the preceding run. (Fig. 26)

(d) All other formulas proved to be more accurate than when used with the greater step length. All of them, however, amplify errors.

(e) The error graphs associated with Formulas 9, 10, 11, 13, 14, 18, 22 and 25 were identical. (Fig. 33)

(3) Increasing the step length to .05 had the following effects:

(a) The formulas which proved best with a step length of .02 are much less accurate with a step length of .05. Figs. 34 through 41 are the error graphs associated with Formulas 6, 10, 11, 12, 13, 15, 22 and 25 using the .05 step length. These graphs show the only formulas retaining any error damping characteristics to be numbers 11, 12 and 25.

b. Program 2800 6

(1) The Coulomb wave Equation was solved for two combinations of values of L and γ ($L=1, \gamma=1$; and $L=2, \gamma=3$), and with various integration step lengths. It was not feasible to generate error graphs for these equations. Fig. 42 lists magnitude of deviation of computed solutions from true values after the number of iterations indicated. The

to limitations of the tables used[3], the minimum error discernable was 1E-7 ($1 = 10^{-7}$). An examination of Fig. 42 reveals the following:

(a) Identical results were obtained in all cases where formulas 9, 13, 14, 15 and 18 were used. This group also produced the most accurate solutions. Reducing step length improved accuracy throughout the range.

(b) Formula 8 solutions were slightly less accurate than those of the group above in solving the equation $y'' + y\left(1-\frac{1}{x}-\frac{1}{x^2}\right) = 0$. Solutions of the equation $y'' + y\left(1-\frac{6}{x}-\frac{6}{x^2}\right) = 0$, using a step length of .02 were more accurate than with any other formula.

6. Conclusions.

In his Numerical Methods[3], Kopal illustrated the shortcomings of going-ahead recursion formulas: those derived from the relationship $y_i = \left\{\frac{h}{\log \epsilon}\right\}^2 Ef_{i-1}$. When using going-across formulas stemming from the integration formula $y_i = \left\{\frac{h}{\log e}\right\}^2 f_i$, an approximation of f_i must be obtained before y_i can be calculated. Therefore, the method suggested by Kopal is essentially the predictor-corrector method coupled with a procedure for deriving an unlimited supply of corrector formulas. Some of these we have seen produce quite accurate solutions to several differential equations of second order. A glance at Figs. 43 - 45, the error of $y'' + y = 0$ after solution by the Milne method, is evidence of the superiority of a number of the correctors derived from Padé convergents.

It is suggested at this point that the less accurate going-ahead type formulas might be generated in the same way and used as predictors.

The fact that certain correctors derived from Padé counterparts perform their tasks as well should provide sufficient motivation for a similar study of predictor derivation.

None of the corrector formulas discussed in this paper are stable for all equations over all ranges of h. Additional formulas could be derived from a polynomial approximation to $\left\{\frac{\log(1-\nabla)}{\nabla}\right\}^{\lambda}$ of higher degree, but this area does not appear promising. In dealing with associated characteristic equations of higher degree it will be extremely difficult to locate values of parameters which will retain all roots within the required bounds.

The excellent results obtained with Formula 15 (Fig. 21) indicate that a fourth degree polynomial approximation to $\left\{\frac{\log(1-\nabla)}{\nabla}\right\}^{\lambda}$ is sufficient to insure that truncation error is not a significant problem. It would seem, therefore, that the use of polynomials of higher degree would invite additional stability complications.

In summary, it is concluded that the procedure suggested by Impel should be viewed as a method of deriving predictor and corrector formulas. The results achieved with some of the correctors derived in this manner indicate that this procedure is promising and merits further study.

7. Recommendations for Future Studies.

a. Investigate the roots of the characteristic equations associated with the more promising recursion formulas discussed in this paper. Ascertain and tabulate values of $\bar{h}$ for which all roots lie within the unit circle. With this data available, one could readily select the best recursion formula for solving a given differential equation over a

specified range of values of the independent variable.

b. Derive a Padé table of rational convergents to $\left\{ \frac{\sin x}{x} \right\}^4$ from which to obtain a number of prime-valued recursion formulas. Substitute each of these in turn for the predictor formula used in Program [5C] 5. Calculate errors and compare with Fig. 4c. In this manner, evaluate the merits of predictor formulas derived from rational Padé convergents. Ralston [6] describes the advantages of using predictors and correctors of the same order.

c. Extend the polynomial representation of $\left\{ \frac{\ln(1+x)}{x} \right\}^2$ beyond seven terms and derive higher order recursion formulas. Investigate the roots of these formulas as suggested in subparagraph a above.

specified range of values of the independent variable.

b. Derive a Padé table of rational convergents to $\left\{ \quad \right\}^{\frac{1}{2}}$ from which to obtain a number of predictor-corrector recursion formulas. Substitute each of these in turn for the predictor formula used in Program TROD 6. Calculate errors and compare with Fig. 32. In this manner, evaluate the merits of predictor formulas derived from rational Padé convergents. Ralston [6] describes the advantages of using predictors and correctors of the same order.

c. Extend the polynomial representation of $\left\{ \frac{\quad}{\sigma} \right\}^{\frac{1}{2}}$ beyond seven terms and derive higher order recursion formulas. Investigate the roots of these formulas as suggested in subparagraph a above.

Fig. 1 - Sample Padé Table

D \ n	0	1	2	3
0	$\frac{1}{1}$	$\frac{1+\nabla}{1}$	$\frac{1+\nabla+\frac{1}{2!}\nabla^2}{1}$	$\frac{1+\nabla+\frac{1}{2!}\nabla^2+\frac{1}{3!}\nabla^3}{1}$
1	$\frac{1}{1-\nabla}$	$\frac{1+\frac{1}{2}\nabla}{1-\frac{1}{2}\nabla}$	$\frac{1+\frac{1}{3}\nabla+\frac{1}{3\cdot 4}\nabla^2}{1-\frac{2}{3}\nabla}$	
2	$\frac{1}{1-\nabla+\frac{1}{2}\nabla^2}$	$\frac{1}{1-\nabla+\frac{1}{6}\nabla^2}$		
3	$\frac{1}{1-\nabla+\frac{1}{2}\nabla^2}$			

Convergents to $\left\{\frac{\log(1-\nabla)}{\nabla}\right\}^2$ derived from third degree polynomial.

The fact that three of the convergents are equal is coincidental.

Fig. 2 - Coefficients of Data Corresponding to $\left\{\frac{\sin(\omega/2)}{\omega}\right\}^2$

No.	Numerator	Denominator
1	1.0	1.0
2	1.0,1.0	1.0
3	1.0,1.0,.917	1.0
4	1.0,1.0,.917,.833	1.0
5	1.0,1.0,.917,.833,.761	1.0
6	1.0,1.0,.917,.833,.761,.700	1.0
7	1.0	1.0,-1.0
8	1.0,.083	1.0,-.917
9	1.0,.091,.008	1.0,-.909
10	1.0,.087,.003,-.004	1.0,-.913
11	1.0,.080,-.003,-.010,-.005	1.0,-.920
12	1.0,.074,-.009,-.016,-.011,-.005	1.0,-.926
13	1.0	1.0,-1.0,.083
14	1.0,0.0	1.0,-1.0,.083
15	1.0,.600,.050	1.0,-.400,-.500
16	1.0,-1.29,-.121,-.014	1.0,-2.29,1.25
17	1.0,-.830,-.082,-.013,-.002	1.0,-1.83,.832
18	1.0	1.0,-1.0,.083
19	1.0,.083	1.0,-.917,.003,.004
20	1.0,-1.0,.050	1.0,-2.0,1.13,-.133
21	1.0,-.954,.077,.002	1.0,-1.95,1.12,-.155
22	1.0	1.0,-1.0,.083,0.0,-.004
23	1.0,-1.0	1.0,-2.0,1.08,-.083,-.004
24	1.0,-1.0,.123	1.0,-2.0,1.21,-.206,.086
25	1.0	1.0,-1.0,.083,0.0,-.004,-.004
26	1.0,-.877	1.0,-1.88,.960,-.073,-.004,-.001

Fig. 3 - Legend of Program Symbols

X	Independent variable
Y	Dependent variable
YP	y'
YDP	y''
YT	$\bar{y}$
ERROR	$\bar{y} - y$
D(I)	$v_I y$
Z(I)	$v_I^1 y$
AN(2)	Coefficient of 2nd numerator term in Padé convergent
AD(4)	Coefficient of 4th denominator term in Padé convergent
AX, AY, AYP, AYDP	Initial values
JP	Number of first convergent to be evaluated ($1 \leq JP \leq$)
JQ	Number of last convergent to be evaluated ($1 \leq JP \leq JQ \leq$)
H	h (integration step length)
N	Number of starting values to be computed by Runge-Kutta method
M	Total number of iterations desired
IN(I)	Denotes number of terms in numerator of formula no. (I). Used for information in printout
ID(I)	Same as IN(I), except refers to denominator terms
DEL(K,I,J)	Array which stores Padé coefficients. K=1 denotes numerator coefficient; K=2, denominator coefficient. I is index no. of convergent. J is the number of a specific term. E.g., DEL(2,7,4) denotes the coefficient of the fourth term in the denominator of convergent no.7.
QO	Coefficient of s_i in recursion formula
Q(J)	Coefficient of s_{i-J} in recursion formula
PO	Coefficient of y''_i in recursion formula
P(J)	Coefficient of y''_{i-J} in recursion formula
L	Index no. of convergent and its associated recursion formula

```
      Fig. 4 (cont'd)
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      [illegible]
  100 CONTINUE
C
C     COMPUTE FIRST AND SECOND DIFFERENCES OF Y
      DO 91 I=2,N
   91 D(I)=Y(I)-Y(I-1)
      DO 92 I=3,N
   92 Z(I)=D(I)-D(I-1)
C
C     SELECT BASE CONVERGENT TO BE USED
      L=JP
C
C     COMPUTE COEFFICIENTS OF RECURSION FORMULA FROM
C     COEFFICIENTS OF BASE CONVERGENT
      AN(1)=1.0
      AD(1)=1.0
  208 CONTINUE
      DO 207 J=2,6
      AN(J)=DEL(1,L,J)
  207 AD(J)=DEL(2,L,J)
   12 QT=0.0
  203 PD=0.0
      DO 14 J=1,6
  202 QQ=QQ+AN(J)
   14 PD=PD+AD(J)
      DO 15 J=1,5
      Q(J)=0.0
      P(J)=0.0
      DO 15 I=J,5
      Q(J)=Q(J)+AN(I+1)*DEL(I,J)
   15 P(J)=P(J)+AD(I+1)*DEL(I,J)
C
      NN=N+1
      DO 17 I=NN,M
C
C     COMPUTE APPROXIMATE VALUE OF Y WITH OTHER PREDICTOR
      Y(I)=Y(I-1)+Y(I-5)-Y(I-4)+(1063/4.0)*(5.0*YDD(I-1)
     1     +2.*YDD(I-2)+5.*YDD(I-3))
      YD=Y(I)-Y(I-1)
C
C     USE RECURSION FORMULA DERIVED FROM BASE CONVERGENTS
C     TO COMPUTE SECOND DIFFERENCES OF Y
      QQ=-Q(1)*Z(I-1)+Q(2)*Z(I-2)-Q(3)*Z(I-3)+Q(4)
     1     *Z(I-4)-Q(5)*Z(I-5)
      PQ=(QQ+YDD(I-1)-P(1)*YDD(I-1)+P(2)*YDD(I-2)-P(3)
     1     *YDD(I-3)+P(4)*YDD(I-4)-P(5)*YDD(I-5))/(1.
      Z(I)=(PQ-QQ)/QQ
```

Fig. 4 (cont'd)

```
*
C     CALCULATE 3 TERM SECOND DIFFERENCE JUST COMPUTED
      D(I)=Z(I)-2.*Q(I-1)
      Y(I)=D(I)+Y(I-1)
   19 ERROR(I)=-Y(I)
*
C     COMPUTE TRUE VALUES OF Y AND CALCULATE ERROR
  210 DO 20 I=1,M
      XI(I)=I
      AI=I
      YT(I)=COSF(H*AI)
   20 ERROR(I)=Y(I)-YT(I)
*
      LABEL=IHCO(L,0,4,IER)
      CALL DRAW (M,XI,ERROR,0,0,LABEL,ITITLE,0.,0.,0.,0.,0.,
     1     5,5,1,LAST)
      IF (L-JQ) 24,25,25
   24 L=L+1
      GO TO 206
   25 PRINT 999
      END
      FUNCTION BINOM (M,N)
      AM=M
      IF (N-0)301,302,302
  302 IF (N-1)303,304,305
  305 IF (M-N)301,303,306
  306 CONTINUE
      K=N-1
      NUM=M
      NONOM=N
      DO 444 I=1,K
      NUM=NUM*(M-I)
  444 NONOM=NONOM*(N-I)
      XNUM=NUM
      XD=NONOM
      BINOM=XNUM/XD
      GO TO 307
  303 BINOM=1.0
      GO TO 307
  304 BINOM=AM
      GO TO 307
  301 PRINT 312
  312 FORMAT (18H BINOM INPUT FAULT)
  307 END
```

Fig. 5 - Program 3000 G (Extended)

```
      DIMENSION A(100),X(2000),RHO(2000),PHI(2000),DPHI(2000),
     1   Y(2000),DY(2000),AY(2000),AYP(2000),ETA(100),
     2   IA(6),B(6),C(6),IT(6)
C
1000  FORMAT (3F10.0)
1001  FORMAT (3I5,2D15.7,2D25.10,2I5,2E15.7)
1002  FORMAT (4D15.8,2D25.16,2D15.8)
1003  FORMAT (1H1,20X,'EIGENVALUE NO. ',I2,5H.  ,
     1   'N =',I5,5H  ETA=,D25.16,
     2   /21X,'ZL=',F4.1//)
1004  FORMAT (I5,I2,2I1,19A4/1X,19A4)
1005  FORMAT (1H1,20X,'EIGENVALUE NO. ',I2,5H.  ,
     1   'N =',I5,
     2   /21X,'ZL=',F4.1//)
1006  FORMAT (E20.7,2X)
1007  FORMAT (1H1,20X,'JOB COMPLETED')
C
C     READ INPUT DATA
      READ 1000, XF, DX
      READ 1001,M,N,MM,IS,IT
      READ 1002, AX,AY,AYP,ETA,ZL,CO
      PRINT 1003, M,N,MM,ETA,ZL
C
C     CONVERT INITIAL VALUES FROM NORMALIZED
C     FORM USED IN MOST TABLES INTO STANDARD FORM
C     DESCRIBED IN THIS PROGRAM AS Y
      LL=ZL
      CL=CO
      DO 201 L=1,LL
  201 CL=(CL*SQRT(ZL**2+ETA**2))/(ZL*(2.*ZL+1.))
      AY=AY*CL*(AX**(LL+1))
      A(LL+1)=1.
      A(LL+2)=ETA/(ZL+1.)
      JL=LL+3
      DO 202 L=JL,100
      XL=L
  202 A(L)=(2.*ETA*A(L-1)-A(L-2))/((XL+ZL)*(XL-ZL-1.))
      PHIS=0.0
      JL=LL+1
      DO 203 L=JL,100
      RL=L
  203 PHIS=PHIS+(L-ZL)*A(L)*AX**(L-LL-1)
      AYP=CL*(PHIS*(ZL+1.)+AX**(LL+1))
C
C     READ PHASE COEFFICIENTS
      DO 11 L=1,97
   11 READ 1004, K,I,(IN(I),ID(I),(DEL(K,I,J),J=2,6))
C
C     COMPUTE N STARTING VALUES BY RUNGE KUTTA METHOD
      Q=DX/2.
      X(1)=XF
      Y(1)=AY
      YP(1)=AYP
      YDP(1)=(-2.*(ZL+1.)*Y(1)-(ETA*(ZL+1.)*Y(1)/X(1)**2)
      I1=IS-1
      I2=IS+2
      DO 101 I=1,I1,N
```

Fig. 3 (cont'd)

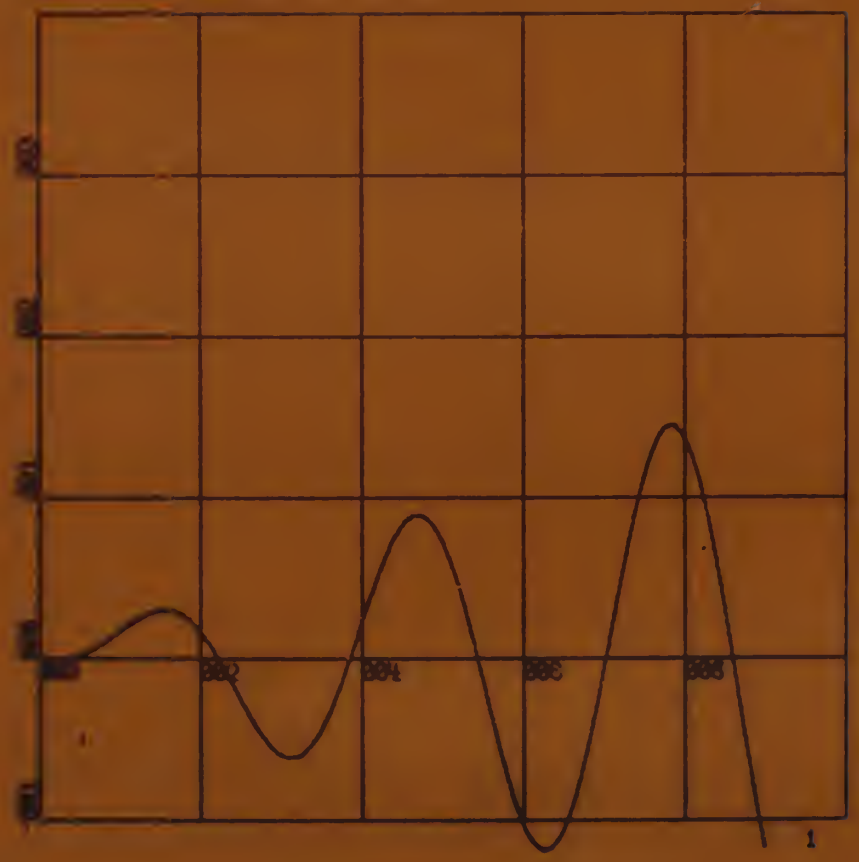
```
      GO TO (101,102),I
      GO TO (1)  0.,2.0*X(1),0.0,0.0,0.0,0.0
  101 DX=X(1)-1.
      X=Y(1-1)
      GO TO 103
  102 X=X(1-1)+DX/2.
      X=X(1-1)+DX/2.+DX*Y(1)/8.
      GO TO 103
  103 X=X(1-1)+H
      DY=Y(1-1)+V+DF(X)
  104 YPP=-DY*(1.-(2.*ETA)/X-(ZL*(ZL+1.))/X**2)
      DY=(YPP/2.)*DX+DY
      AVT=(DY(1)+DY(2)+DY(3))/3.
      DY=(DY(1)+3.*DY(2)+3.*DY(3)+DY(4))/8.
      X(I)=X(I-1)+H
      Y(I)=Y(I-1)+V+DKT
      V=V+DKP
      YP(I)=V/H
  105 YDF(I)=-Y(I)*(1.-(2.*ETA)/X(I)-(ZL*(ZL+1.))/X(I)**2)
*
C     COMPUTE FIRST AND SECOND DIFFERENCES OF Y
      DO 106 I=IS1,N
  106 D(I)=Y(I)-Y(I-1)
      DO 107 I=IS2,N
  107 E(I)=D(I)-D(I-1)
*
C     SELECT PADE CONVERGENT TO BE USED
      L=JP
*
C     COMPUTE RECURSION FORMULA COEFFICIENTS FROM PADE
C     COEFFICIENTS
      AN(1)=1.0
      AD(1)=1.0
  108 CONTINUE
      DO 109  J=2,6
      AN(J)=DEL(1,L,J)
  109 AD(J)=DEL(2,L,J)
      QQ=0.0
      PQ=0.0
      DO 110 J=1,6
      QQ=QQ+AN(J)
  110 PQ=PQ+AD(J)
      DO 111 J=1,5
      Q(J)=AN(J)
      P(J)=AD(J)
      DO 111 I=J,5
      Q(J)=Q(J)+AN(I+1)*X(I-J)*DM(I,J)
  111 P(J)=P(J)+AD(I+1)*X(I-J)*DM(I,J)
*
      NNN=I
      DO 112 I=NNN,N
      X(I)=X(I-1)+H
*
C     OBTAIN FIRST APPROXIMATION TO Y  BY USING MILNE PREDICTOR
```

Fig. 5 (cont'd)

```
C
C     OBTAIN INTERPOLATED VALUE OF SECOND DIFFERENCE OF Y
C     USING FORMULA DERIVATED FROM BASIC CONSTRUCTS
      DF=DY(I)+(DY(I+1)-DY(I))*(X-X(I))/(X(I+1)-X(I))
     1   -DY(I)*(X-X(I))/(X(I+1)-X(I))
      D2=2.*(DY(I+1)-DY(I))/(X(I+1)-X(I))
      IF(I.EQ.1) GO TO 107
C
C     COMPUTE Y FROM DIFFERENCES JUST CALCULATED
      DY(I)=Z(I)*DX+DY(I-1)
      Y(I)=Y(I-1)+DY(I-1)+.5*(DX**2)*D2
  107 YDOT(I)=Y(I-1)+(2.*DX)/3.*(1.-(ZL*(ZL+1.)/6.)*DX**2)
C
C     CONVERT ALL COMPUTED VALUES OF Y INTO
C     NORMALIZED FORM FOR COMPARISON WITH STANDARD TABLES
      DO 200 I=NN,M
  200 X(I)=Y(I)/((ZL*(ZL+1.))**(ZL+1.))
      PRINT 1005,L,(DY(L),DD(L))
      PRINT 1006,(Y(I),I=15,M,IT)
      IF(L-20) 113,114,114
  113 L=L+1
      GO TO 108
  114 PRINT 1007
      END
      FUNCTION BINOM (M,N)
      BM=1
      IF(N-M/2) 201,201,202
  201 IF (N-1) 205,205,203
  202 IF (M-N-1) 204,205,203
  203 K=N-1
      NUM=M
      NUM=NUM*
      DO 206 I=1,K
      NUM=NUM*(M-I)
  206 DENOM=DENOM*(J-I)
      BINOM=NUM/DENOM
      GO TO 208
  204 BINOM=M
      GO TO 208
  205 BINOM=1.
      GO TO 208
  207 PRINT 1000
 1000 FORMAT (1H0 ERROR INPUT FAULT)
      STOP
  208 END
```

Fig. 5 - Relation of Formula Numbers to Pade Convergents

Formula	Degree of Convergent (N/D)	Formula	Degree of Convergent (N/D)
1	0/0	14	1/2
2	1/0	15	2/2
3	2/0	16	3/2
4	3/0	17	4/2
5	4/0	18	0/3
6	5/0	19	1/3
7	0/1	20	2/3
8	1/1	21	3/3
9	2/1	22	0/4
10	3/1	23	1/4
11	4/1	24	2/4
12	5/1	25	0/5
13	0/2	26	1/5

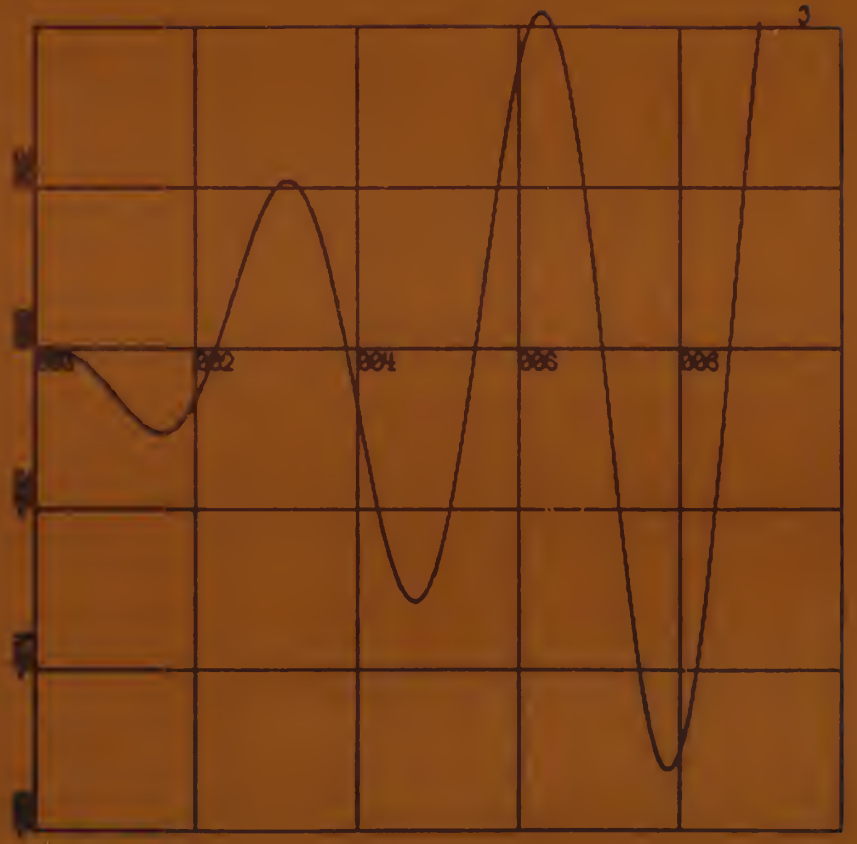


X-SCALE - LAMBDA/2 UNITS/DIVISION
Y-SCALE - LAMBDA/4Π UNITS/DIVISION

W.L.BUMOYE, THESIS. ERROR VS L

Fig. 8 - Formula 2 Error
Step Length = .05

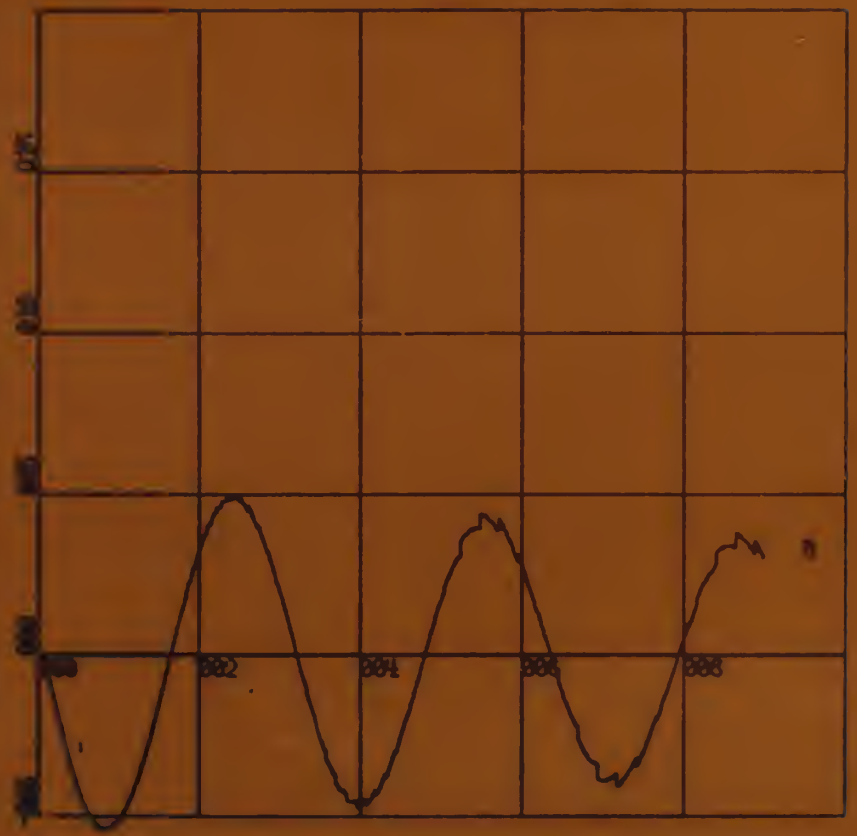
W.BUMOYE, THESIS, ERROR VS L.



W.B.MOYE, THESIS. ERROR VS I.

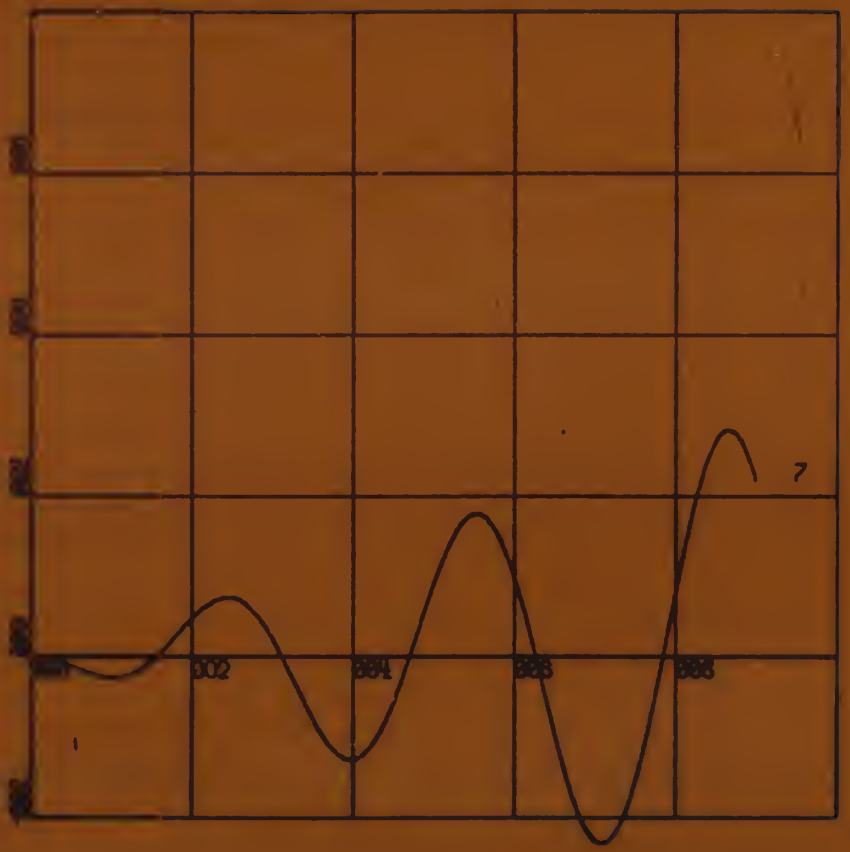
Fig. 10 - Formula 6 Error
Step length = .01

Fig. 11 - Formula 5 Error
Step Length = .05



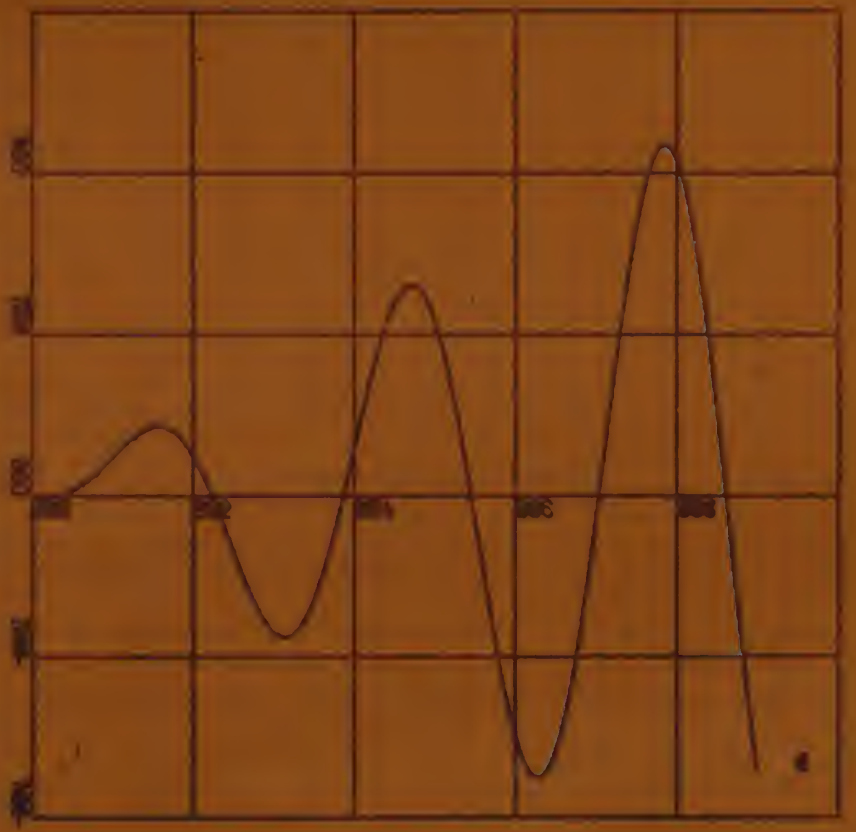
X-SCALE - CARET=.40 UNITS/INCH
Y-SCALE - CARET=.10 UNITS/INCH

W.L.BUMOYE, THESIS. ERROR VS L



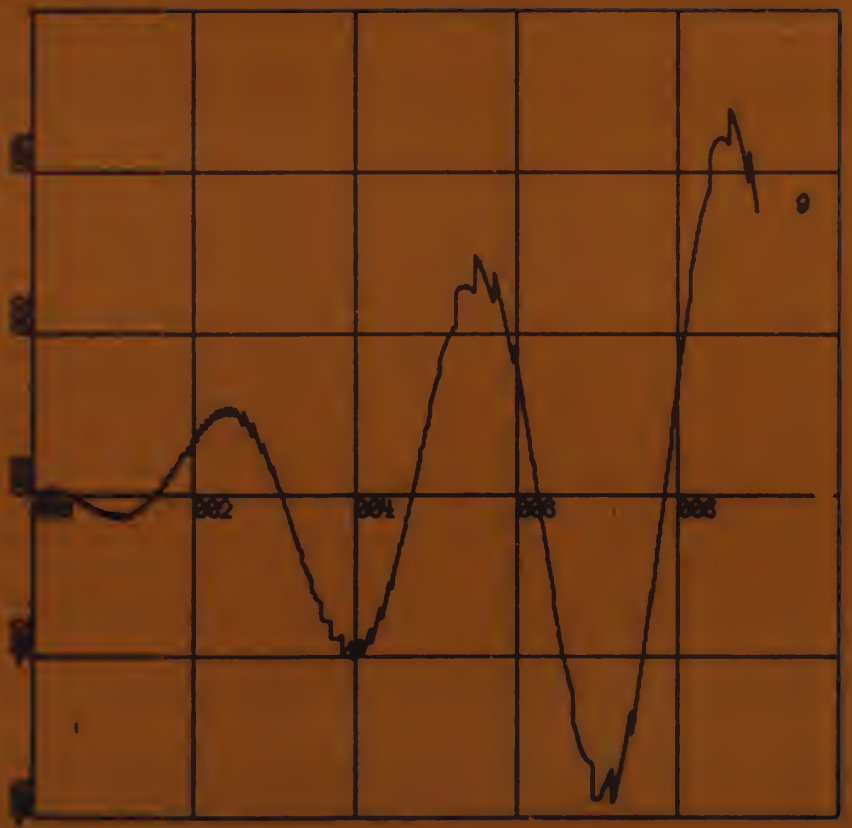
X-SCALE - [illegible] UNITS/INCH
Y-SCALE - [illegible] UNITS/INCH

W.L.BUMOYE, THESIS. ERROR VS L.



X-SCALE - [illegible]
Y-SCALE - [illegible]

W.L.B.MOYE, THESIS. ERROR VS I.



W.L.&.MOYE, THESIS. ERROR VS L

Fig. 16 - Formula 10 Error
Step Length = .02

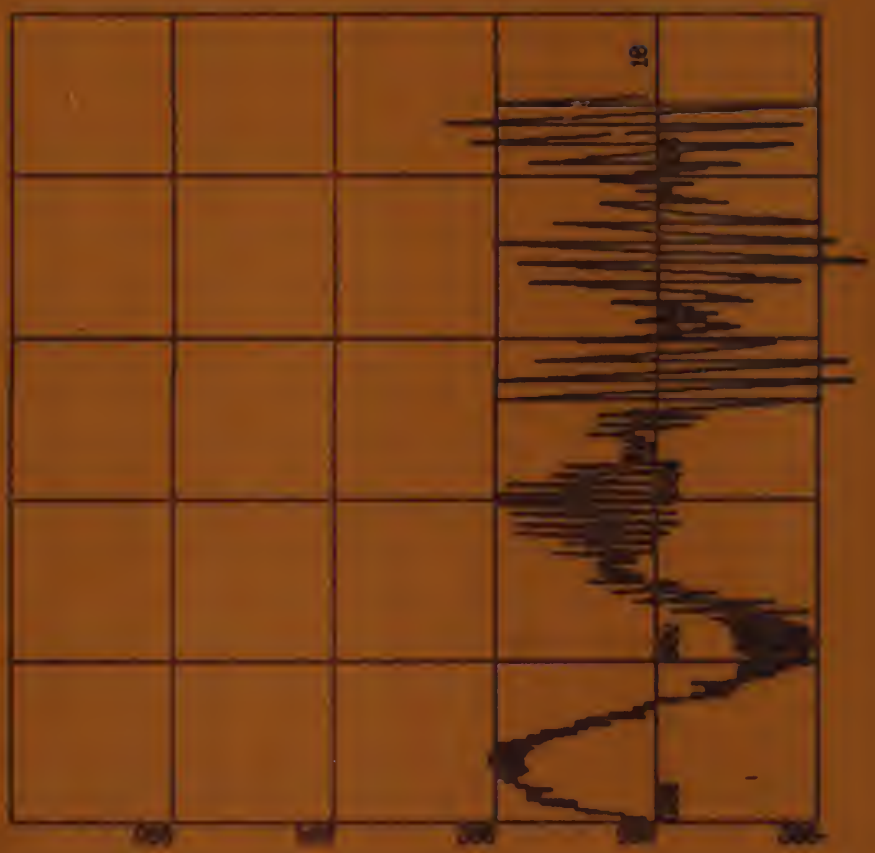
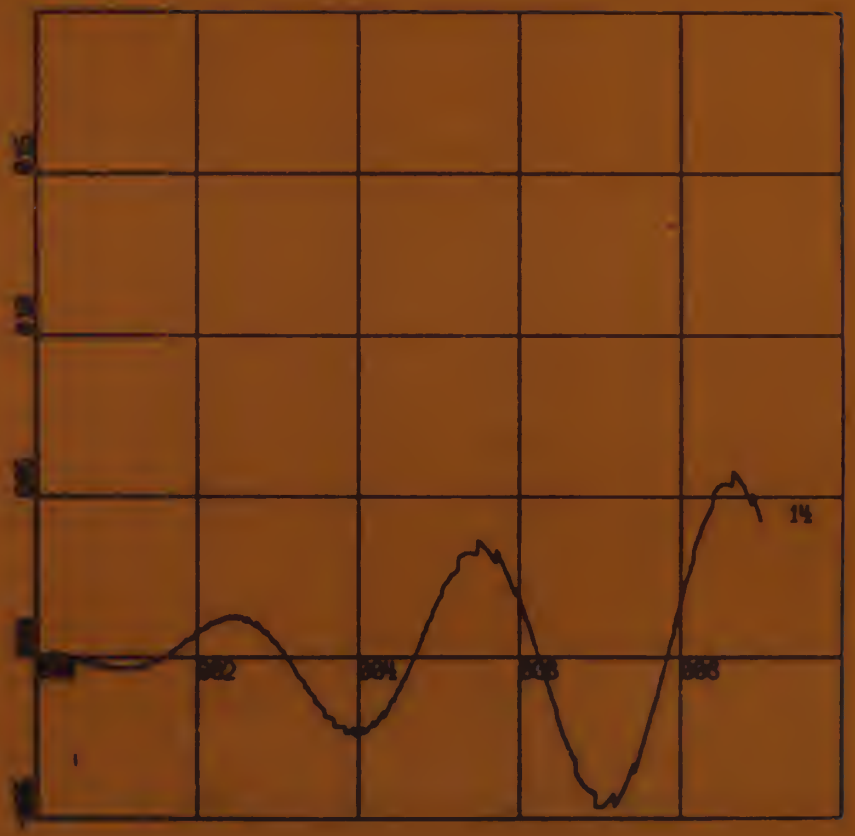


Fig. 17 - Formula 11 Error
Step Length = .02

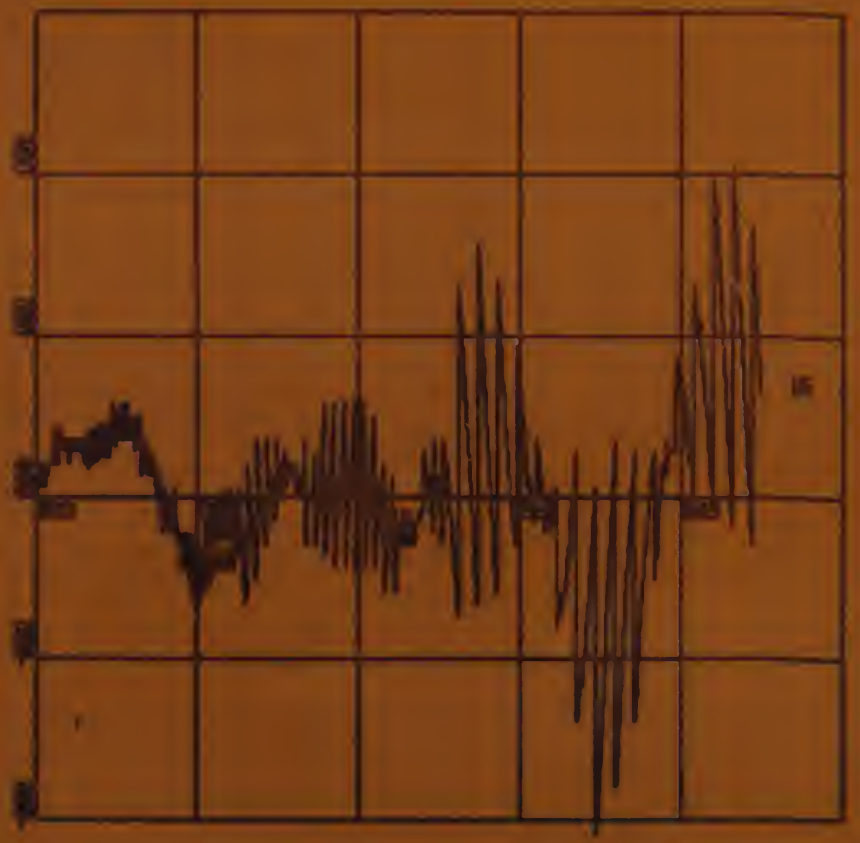
Fig. 18 - Formula 12 Error
Step Length = .01

Fig. 17 - Formula 13 Error
Step Length = .04



X-SCALE - SAME AS UNITS/INCH
Y-SCALE - SAME AS UNITS/INCH

WLELMOYE, THESIS, ERROR VS I.

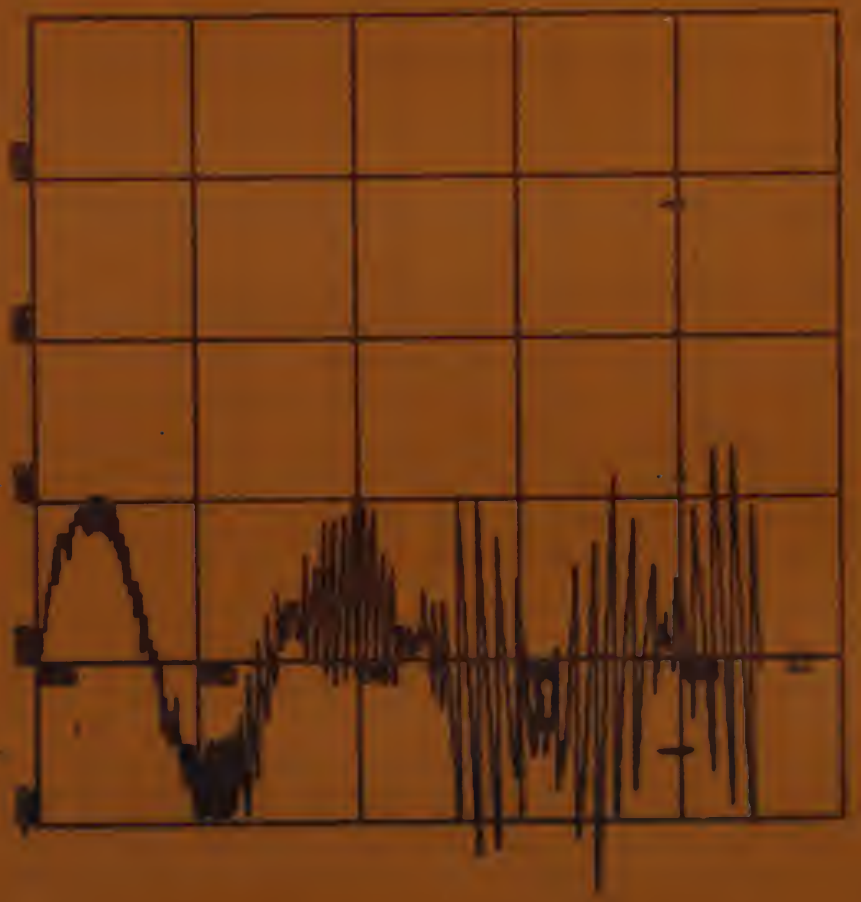


X-SCALE - [illegible]
Y-SCALE - [illegible]

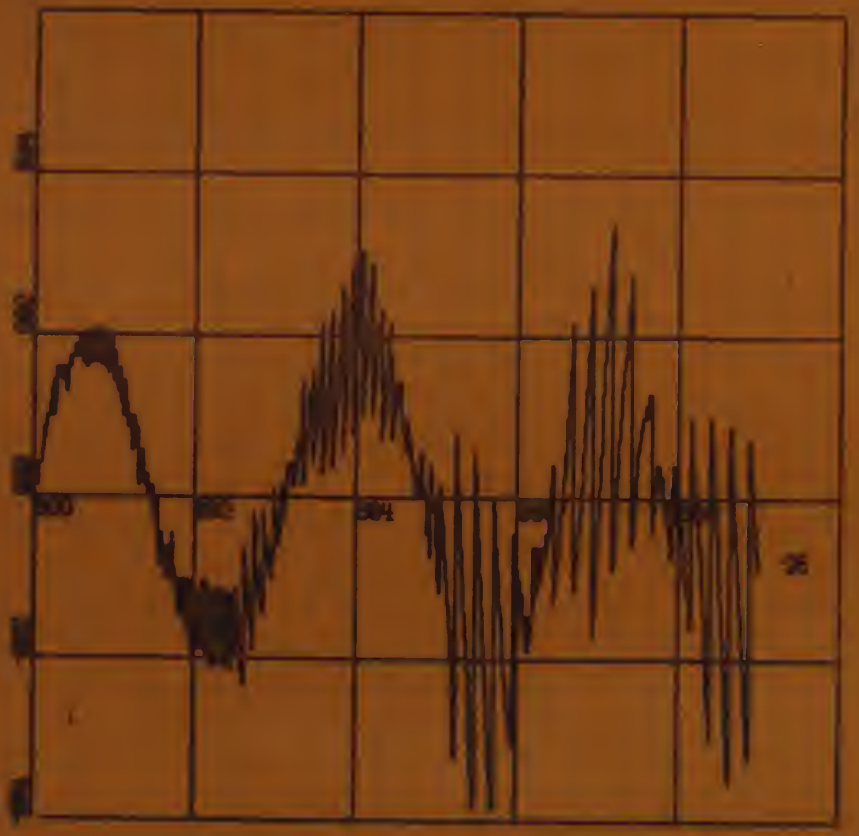
L.L.BUMOYE. THESIS. ERROR VS T.

Fig. 27 - Formula 18 Error
Step Length = .03

Fig. 10 - Parabolic 10 Banner
Step Length = .02

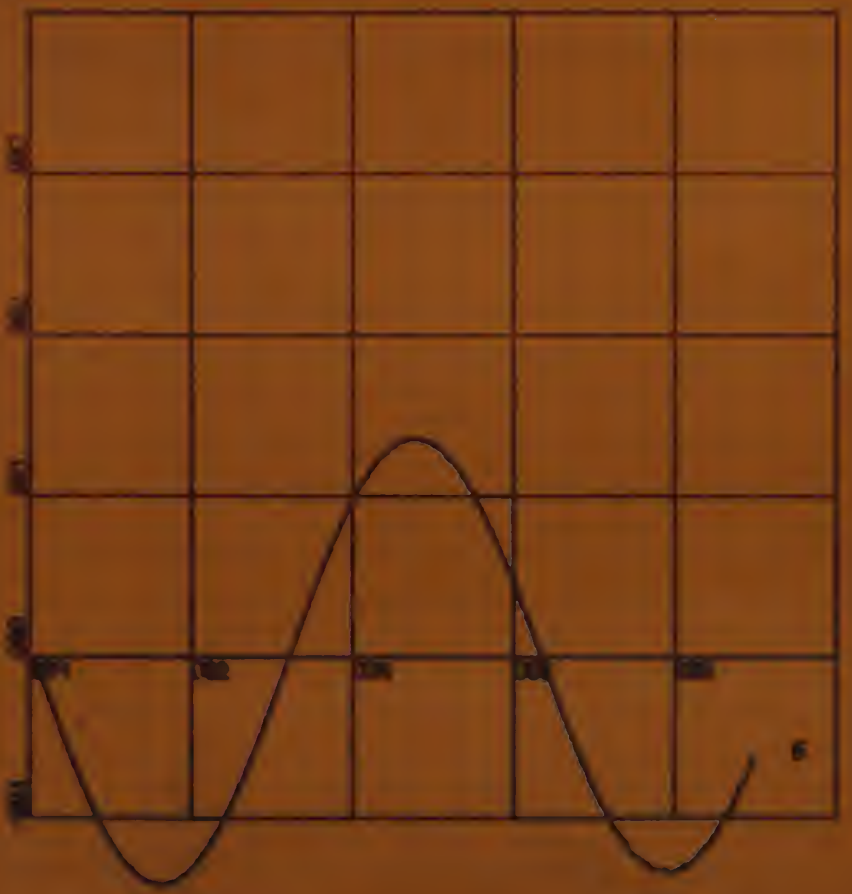


WLBMOYE, THESIS. ERROR OS L.

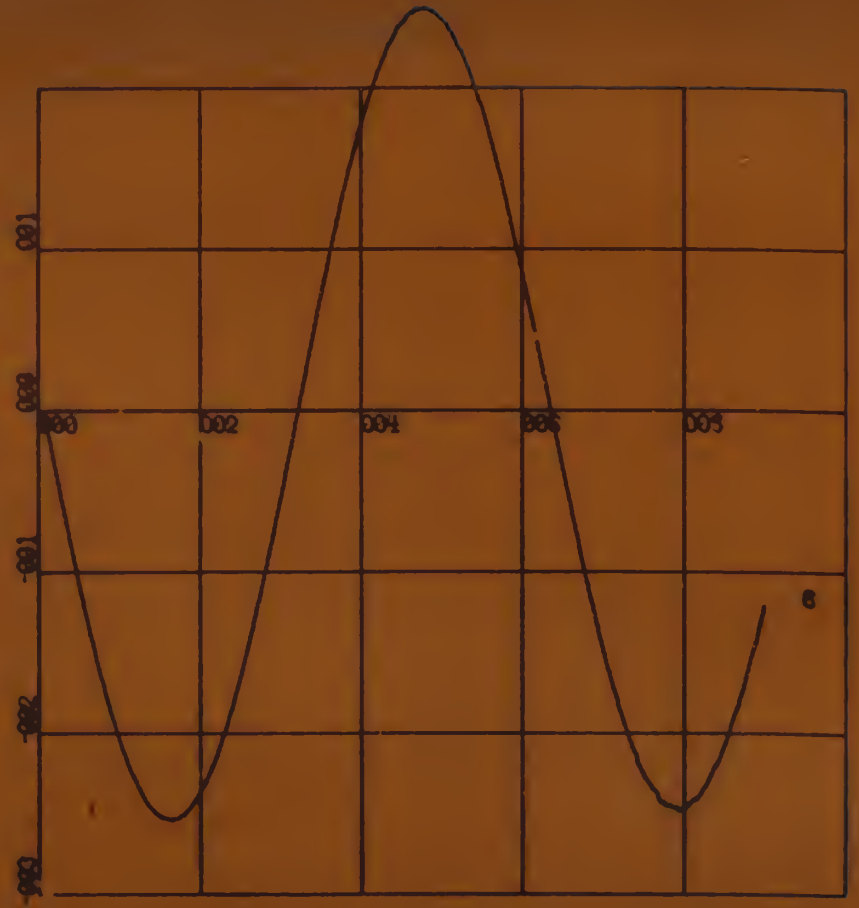


X-SCALE - [illegible]
Y-SCALE - [illegible]

W.L.&J.MOYE, THESIS. ERROR VS I.

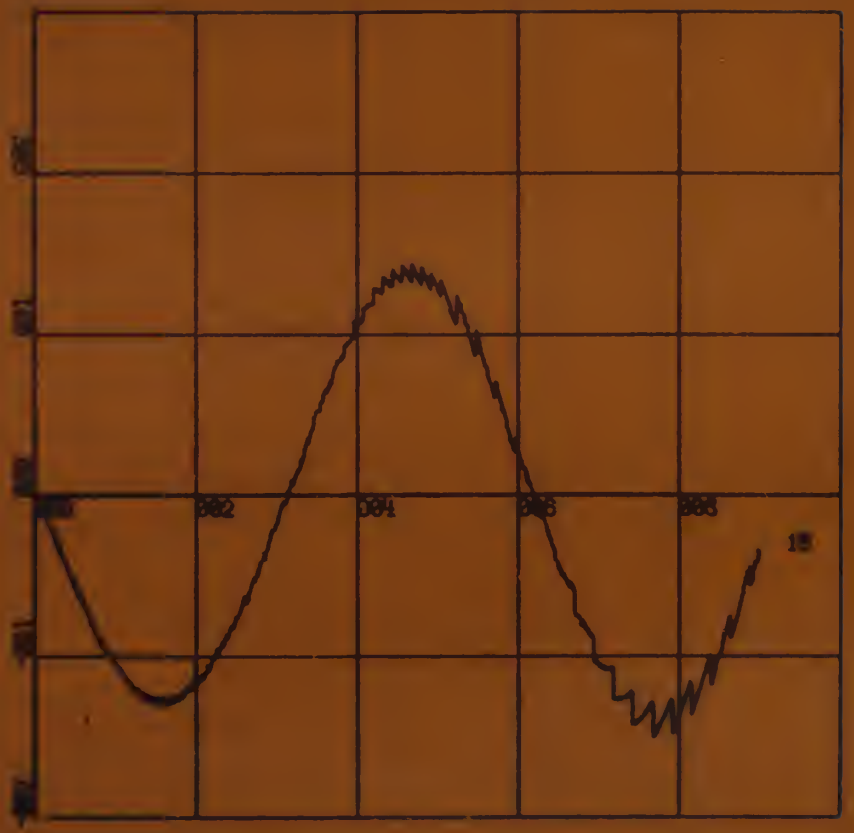


W.BUMDYE. THESIS. ERROR VS I.



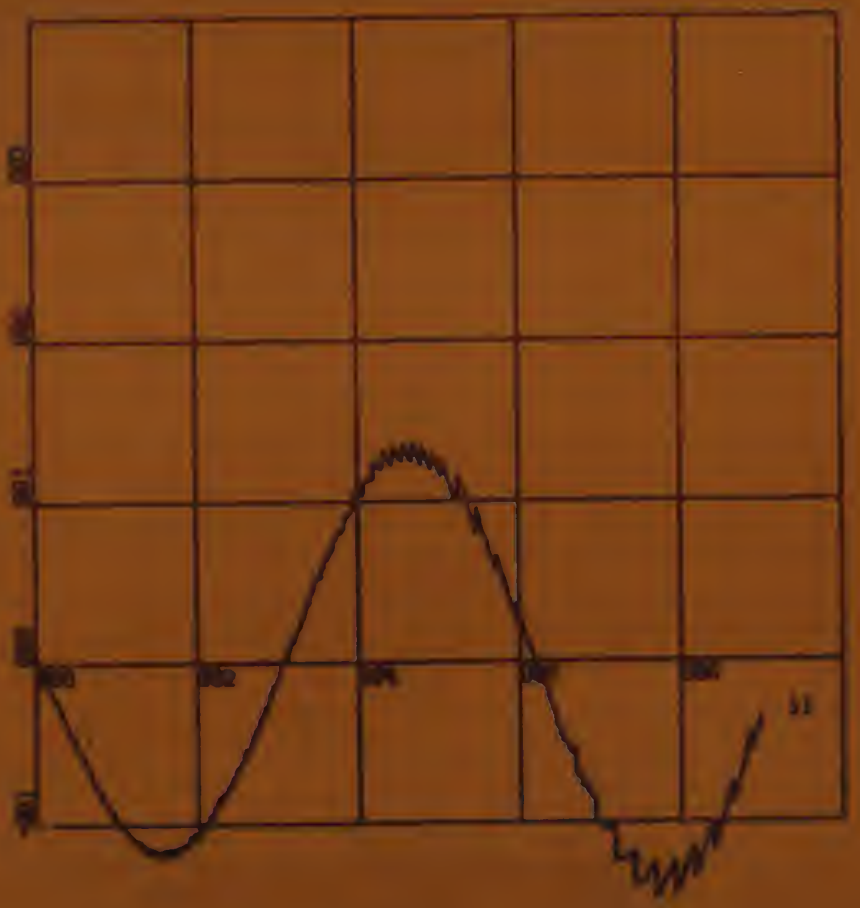
X-SCALE - .1 UNITS=1 INCH
Y-SCALE - .1 UNITS=1 INCH

WLBJMOYE, THESIS. ERROR VS 1.



X-SCALE - [illegible] UNITS/INCH
Y-SCALE - [illegible] UNITS/INCH

W.L.B.J.MOYE, THESIS. ERROR VS I.



W.E.B.MOYE. THESIS. ERROR VS I.

Fig. 37 - Formula 17 Error
Step Length = .01

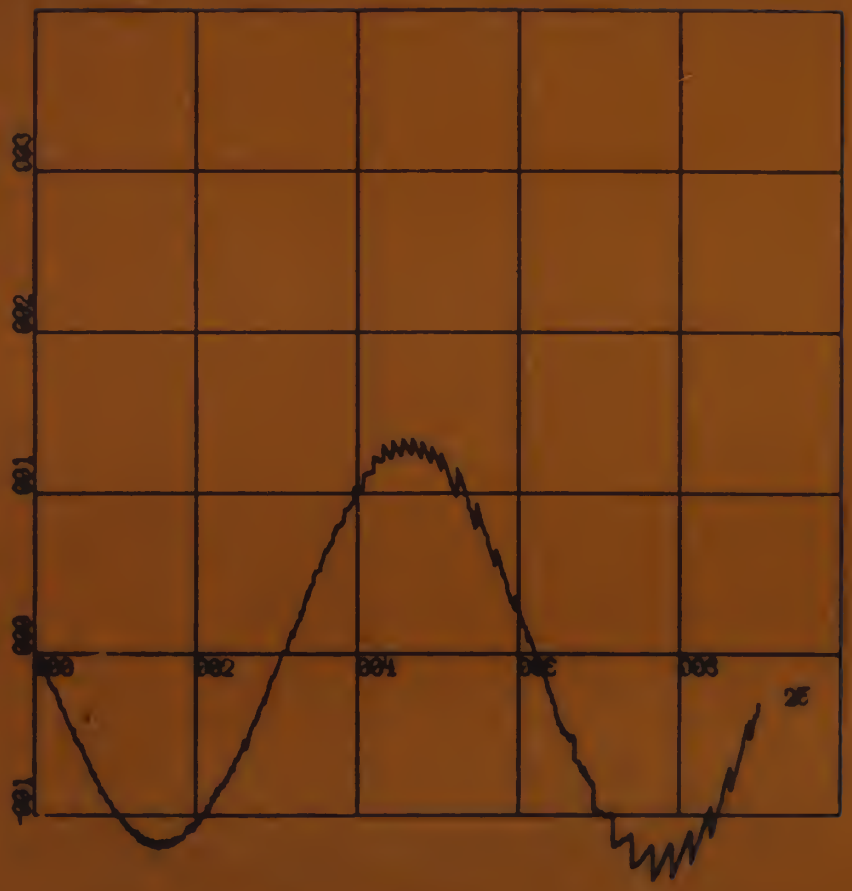
X-SCALE - SIMPSON INTEGRATION
Y-SCALE - GAUSS-LEGENDRE INTEGRATION
WILDMOYE, THESIS, ERROR VS I.

Fig. 31 - Formula L1 Error
Step Length = .01

WILMORE, THESIS, ERROR VS L

Fig. 37 - Formula 22 Error
Step Length = .31

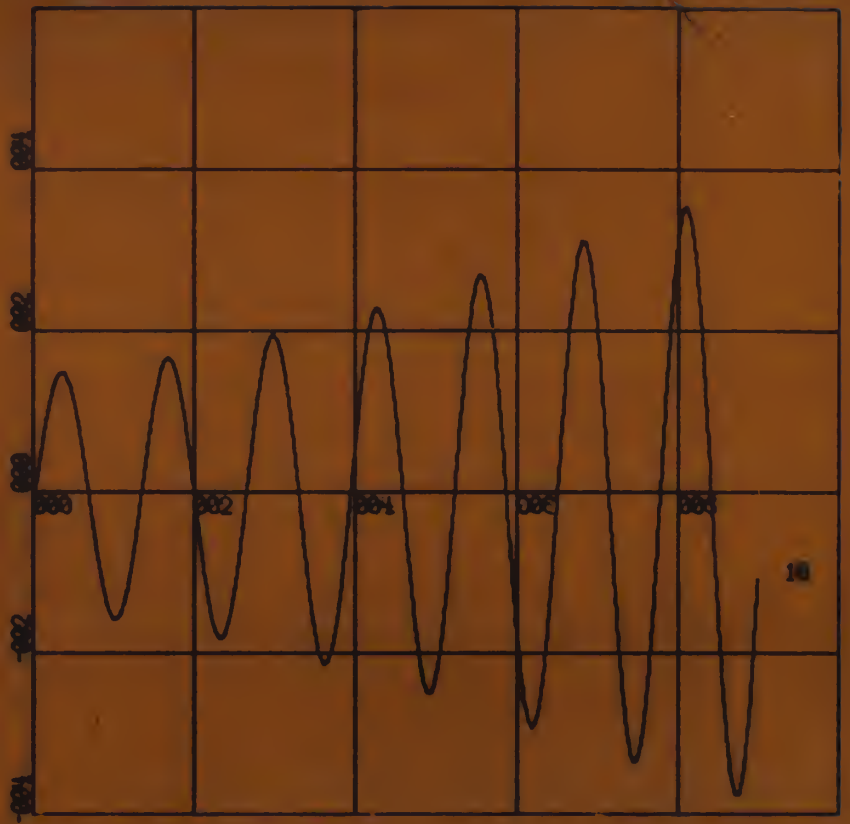
THESIS - UNIVERSITY OF ILLINOIS
THESIS - UNIVERSITY OF ILLINOIS
WAMIYE, THESIS, ERROR US 1



W.B.MOYE, THESIS. ERROR VS L

Fig. 11 - Formula 6 Error
Step Length = .05

W.B.MOYE, THESIS, ERROR VS I.



X-SCALE - 2.000-400 UNITS/INCH
Y-SCALE - 2.000-10 UNITS/INCH

W.B.MOYE, THESIS. ERROR VS I.

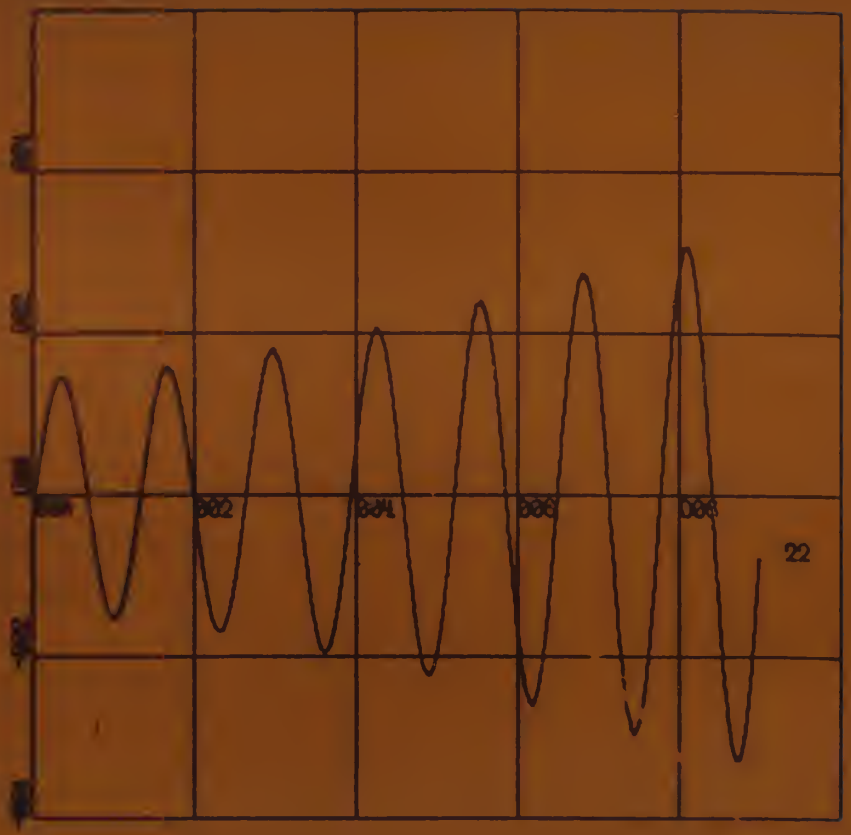
Fig. 3E - Formula 11 Error
Plot Length = .05

X-MODULE - [illegible] UNITS/INCH
Y-MODULE - [illegible] UNITS/INCH

W.B.MOYE, THESIS. ERROR VS I.

Fig. 3F - Formula 15 Error
Step Length = .05

X-SCALE - 2.00E+02 UNITS/INCH
Y-SCALE - 2.00E-03 UNITS/INCH
W.B.MOYE, THESIS. ERROR VS I.

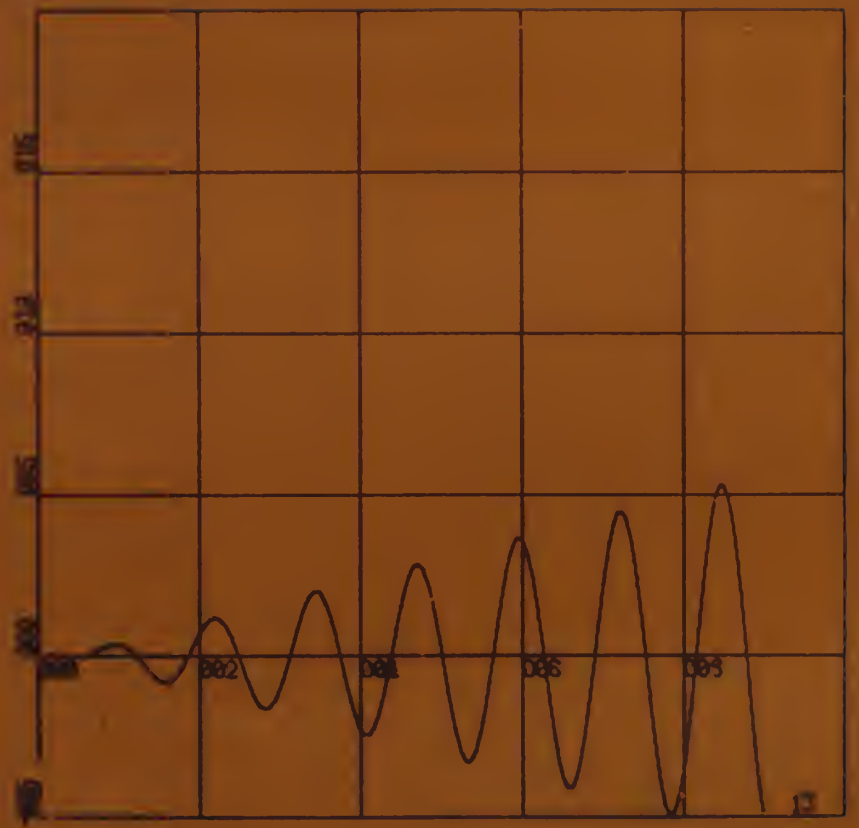


Y-SCALE - 2.00E+00 UNITS/DIV.
T-SCALE - 2.00E-06 UNITS/DIV.

W.L.B.MOYE, THESIS. ERROR VS I.

X-SCALE - .0002 UNITS/DIVISION
Y-SCALE - .001 UNITS/DIVISION

W.B.MOYE, THESIS. ERROR VS I.

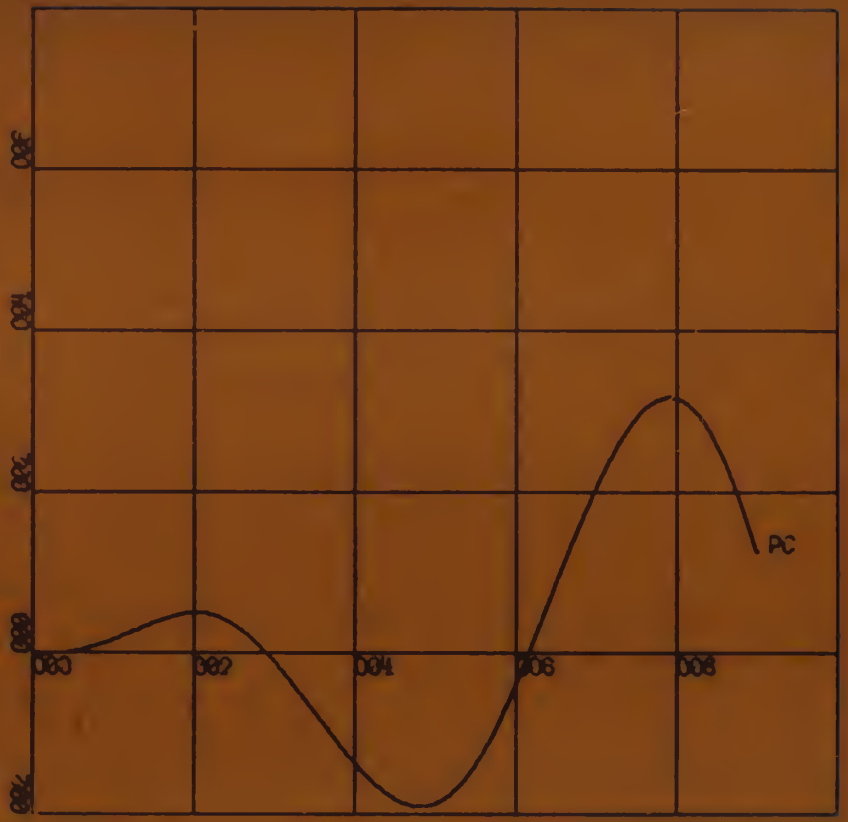


W.B.MOYE, THESIS. ERROR VS I.

Fig. 42 - Solution error; Coulomb Wave Equations

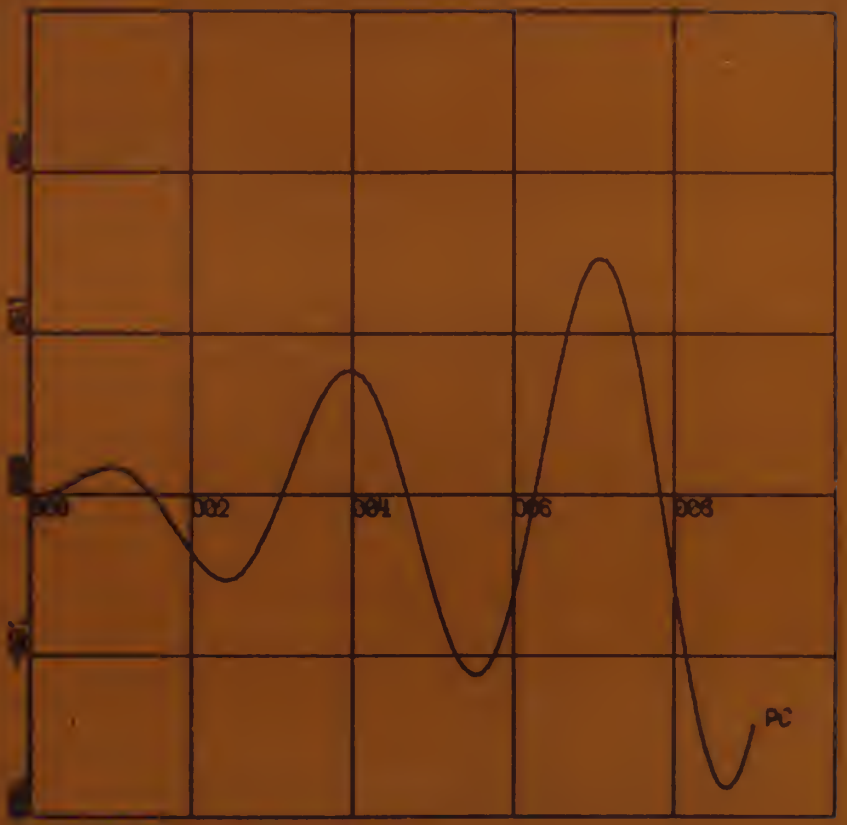
Equations	$y'' + y(1 - 2/x - 2/x^2) = 0$				$y'' + y(1 - 2/x - 2/x^2) = 0$			
Step	.01	.02	.05	.1	.01	.02	.05	.1
Formula No.								
1	9E-3	2E-1	4E-2	8E-1	5E-1	----	----	----
2	5E-5	2E-3	1E-2	3E-3	4E-3	2E-2	5E-2	1E-1
3	4E-7	3E-5	5E-5	5E-4	9E-6	6E-5	3E-4	2E-3
4	----	----	----	----	----	----	----	----
5	----	----	----	----	----	----	----	----
6	----	----	----	----	----	----	----	----
7	5E-7	2E-4	9E-5	2E-4	3E-4	1E-3	5E-3	1E-2
8	0	0	4E-7	4E-6	0	0	3E-5	5E-4
9	0	0	0	1E-7	0	1E-7	3E-5	5E-4
10	7E-4	5E-3	4E-4	4E-4	2E-1	2E-1	9E-2	1E-1
11	3E-3	2E-2	6E-6	1E-3	8E-1	8E-1	7E-1	6E-1
12	----	----	----	----	----	----	----	----
13	0	0	0	1E-7	0	1E-7	3E-5	5E-4
14	0	0	0	1E-7	0	1E-7	3E-5	5E-4
15	0	0	0	1E-7	0	1E-7	3E-5	5E-4
18	0	0	0	1E-7	0	1E-7	3E-5	5E-4
19	7E-4	5E-3	7E-5	5E-4	3E-1	2E-1	2E-1	2E-1
22	3E-2	3E-3	4E-4	1E-3	2E-1	2E-1	2E-1	2E-1
25	2E-3	1E-2	5E-4	3E-3	7E-1	7E-1	1E-5	3E-1
Iterations	400	200	80	40	400	200	80	40

Tabulated values are final solution error after number of iterations indicated. Dashes indicate error in excess of 1E+0 (1×10^{0}).

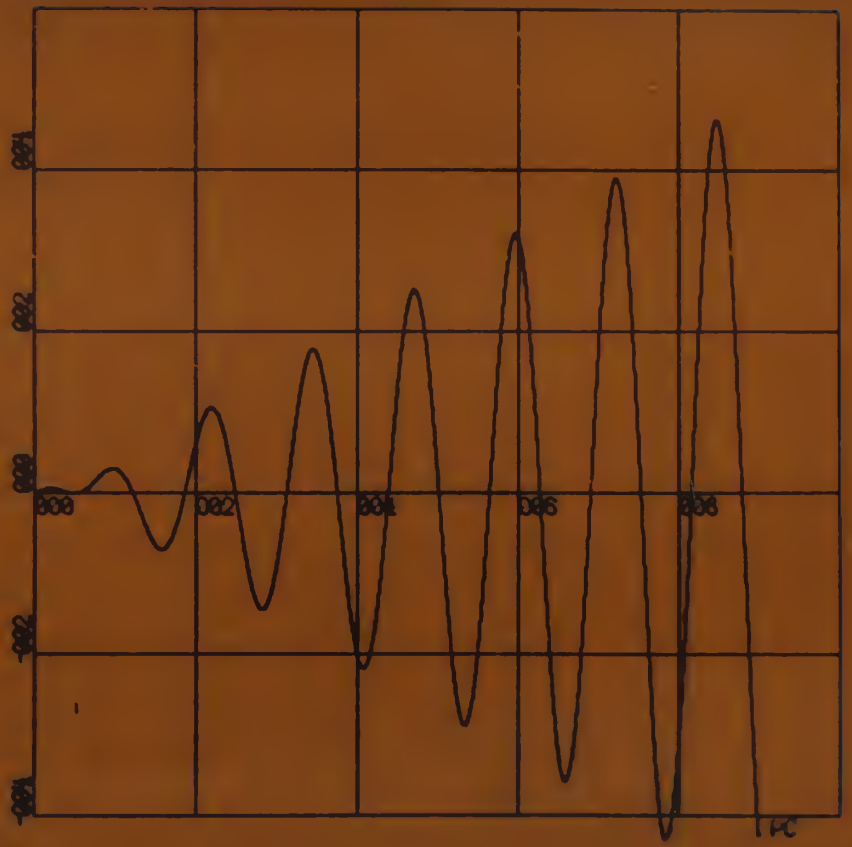


Y-SCALE - .2000+02 UNITS/INCH
X-SCALE - .2000+00 UNITS/INCH

W.B.MOYE, THESIS. ERROR VS I.



W.L.B.MOYE, THESIS. ERROR VS I.



X-SCALE - [illegible]
Y-SCALE - [illegible]

W.B.MOYE, THESIS. ERROR VS I.

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U. S. Naval Postgraduate School Monterey, California	Unclassified N/A

3 REPORT TITLE

NUMERICAL SOLUTION OF SECOND ORDER DIFFERENTIAL EQUATIONS USING RATIONAL PADE' CONVERGENTS.

4 DESCRIPTIVE NOTES (Type of report and inclusive dates)

Thesis for the Master of Science Degree in Mathematics.

5 AUTHOR(S) (Last name, first name, initial)

MOTE, William B. Jr., LCDR, USN

6 REPORT DATE	7a TOTAL NO. OF PAGES	7b NO. OF REFS
March, 1966	61	6

8a CONTRACT OR GRANT NO	9a ORIGINATOR'S REPORT NUMBER(S)
N/A b. PROJECT NO N/A c. N/A d. N/A	N/A 9b. OTHER REPORT NO(S) (Any other numbers that may be assigned this report) N/A

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Rational Pade' convergents to a function of the forward shift operator E are computed from coefficients of its power series expansion. These Pade' convergents are used to generate recursion formulas which are then employed to obtain approximate numerical solutions of several second order differential equations. A variety of integration step lengths are used. Solution error is plotted against the number of iteration steps and results are evaluated. It is concluded that this procedure is beneficial as a method of deriving corrector formulas to be used in the predictor-corrector method of solving second order differential equations. A method for deriving improved predictor formulas is suggested.

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KEY WORDS	LINK A		LINK B		LINK C	
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Numerical Solution						
Second Order Differential Equations						
Linear Multistep Method						
Computed Results.						

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